

METHOD CONTROL PARAMETERS

Method Information For: C:\MSDCHEM\1\METHODS (b) (7)
(C) RP1581_Fatty Acids.M
Method Sections To Run:

() Save Copy of Method With Data
() Instrument Control Pre-Run Cmd/Macro =
() Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
(X) Data Analysis
() Instrument Control Post-Run Cmd/Macro =
() Data Analysis Post-Run Cmd/Macro =
Method Comments:

END OF METHOD CONTROL PARAMETERS

INSTRUMENT CONTROL PARAMETERS: Instrument 1

C:\MSDCHEM\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Thu Jun 26 13:42:00 2014 (C)

Control Information

Sample Inlet : GC
 Injection Source : GC ALS
 Mass Spectrometer : Enabled

Oven
 Equilibration Time 0.5 min
 Oven Program On
 50 °C for 2 min
 then 25 °C/min to 170 °C for 0 min
 then 4 °C/min to 211 °C for 0 min
 then 10 °C/min to 300 °C for 4 min
 Run Time 29.95 min

Front Injector
 Syringe Size 10 µL
 Injection Volume 1 µL
 Injection Repetitions 1
 Solvent A Washes (PreInj) 2
 Solvent A Washes (PostInj) 3
 Solvent A Volume 8 µL
 Solvent B Washes (PreInj) 2
 Solvent B Washes (PostInj) 3
 Solvent B Volume 8 µL
 Sample Washes 1
 Sample Wash Volume 8 µL
 Sample Pumps 3
 Dwell Time (PreInj) 0 min
 Dwell Time (PostInj) 0 min
 Solvent Wash Draw Speed 300 µL/min
 Solvent Wash Dispense Speed 6000 µL/min
 Sample Wash Draw Speed 300 µL/min
 Sample Wash Dispense Speed 6000 µL/min
 Injection Dispense Speed 6000 µL/min
 Viscosity Delay 0 sec
 Sample Depth Disabled

Back Injector

Front SS Inlet He
 Mode Splitless
 Heater On 250 °C
 Pressure On 26.568 psi
 Total Flow On 34.2 mL/min
 Septum Purge Flow On 3 mL/min
 Gas Saver On 20 mL/min After 5 min
 Purge Flow to Split Vent 30 mL/min at 2.5 min

Back SS Inlet He
 Mode Split
 Heater Off
 Pressure Off
 Total Flow Off
 Septum Purge Flow Off
 Gas Saver Off

Split Ratio 100 :1
Split Flow 0 mL/min

Thermal Aux 2 {MSD Transfer Line}
Heater On
Temperature Program On
280 °C for 0 min
Run Time 29.95 min

Column #1
HP-5MS UI: 2689.34800
HP-5MS UI
325 °C: 20 m x 180 µm x 0.18 µm
In: Front SS Inlet He
Out: Front Detector µECD

(Initial) 50 °C
Pressure 26.568 psi
Flow 1.2 mL/min
Average Velocity 41.782 cm/sec
Holdup Time 0.79779 min
Flow Program On
1.2 mL/min for 0 min
Run Time 29.95 min

Front Detector µECD
Heater On 300 °C
Anode Flow Off
Makeup Flow On 20 mL/min
Const Col + Makeup Off
Electrometer Off

Aux Pressure 1 He
Pressure Program Off
10 psi for 0 min
Run Time 29.95 min

Aux Pressure 2 He
Pressure Program Off
10 psi for 0 min
Run Time 29.95 min

Aux Pressure 3 He
Pressure Program Off
10 psi for 0 min
Run Time 29.95 min

Signals
Front Signal Save Off
Back Inlet Save Off
Test Plot Save Off
Test Plot Save Off

MS ACQUISITION PARAMETERS

General Information

Tune File : dftppnew061214.u
Acquisition Mode : Scan

MS Information

Solvent Delay : 4.00 min

EMV Mode : Relative
Relative Voltage : -71
Resulting EM Voltage : 1529

[Scan Parameters]

Low Mass : 35.0
High Mass : 500.0
Threshold : 50
Sample # : 3 A/D Samples 8
Plot 2 low mass : 50.0
Plot 2 high mass : 550.0

[MSZones]

MS Source : 230 C maximum 250 C
MS Quad : 150 C maximum 200 C

END OF MS ACQUISITION PARAMETERS

TUNE PARAMETERS for SN: US73347311

Trace Ion Detection is OFF.

EMISSION : 34.610
ENERGY : 69.922
REPELLER : 23.422
IONFOCUS : 90.157
ENTRANCE_LE : 0.000
EMVOLTS : 1600.000

Actual EMV : 1529.41
GAIN FACTOR : 0.60

AMUGAIN : 2086.000
AMUOFFSET : 128.750
FILAMENT : 1.000
DCPOLARITY : 0.000
ENTLENDOFFS : 18.573@ 3 18.573@ 50 13.804@ 69 12.800@131 13.051
@219 13.553@414 13.302@502 13.302@1049
MASSGAIN : -460.000
MASSOFFSET : -40.000

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL PARAMETERS

DATA ANALYSIS PARAMETERS

Method Name: C:\MSDCHEM\1\METHODS\ (b) (7) RP1581_Fatty Acids.M

Percent Report Settings

Sort By: Signal

Output Destination

Screen: No
Printer: No
File: No

Integration Events: Meth Default

Generate Report During Run Method: Yes

Signal Correlation Window: 0.020

Qualitative Report Settings

Peak Location of Unknown: Apex

Library to Search Minimum Quality
C:\Database\NIST05a.L 0

Integration Events: Meth Default

Report Type: Summary

Output Destination

Screen: No
Printer: No
File: No

Generate Report During Run Method: Yes

Quantitative Report Settings

Report Type: Detailed

Output Destination

Screen: No
Printer: Yes
File: No

Generate Report During Run Method: No

RP1581_DBH_Fatty Acids_ & MCHM

Calibration Last Updated: Mon Jun 23 11:10:12 2014

Reference Window: 2.00 Minutes

Non-Reference Window: 1.00 Minutes

(b) (7) (C) RP1581_Fatty Acids.M Thu Jun 26 13:41:59 2014

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Correlation Window: 0.10 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

1) Octanoic Acid

()

Ret. Time 5.495 min., Extract & Integrate from 4.995 to 5.995 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-------------|-----------|----------------|----------------------|
| Tgt 60.00 / | | | *** METH DEFAULT *** |
| Q1 73.10 / | 59.10 | 20.0 | *** METH DEFAULT *** |
| Q2 101.10 / | 20.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 2.010 / | 17126 |
| 2 | 5.020 / | 72752 |
| 3 | 7.530 / | 134541 |
| 4 | 10.040 / | 188369 |
| 5 | 20.080 / | 436689 |
| 6 | 40.160 / | 922605 |

Qualifier Peak Analysis ON
Curve Fit: Linear

2) Decanoic Acid

()

Ret. Time 6.598 min., Extract & Integrate from 6.098 to 7.098 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-------------|-----------|----------------|----------------------|
| Tgt 60.10 / | | | *** METH DEFAULT *** |
| Q1 73.10 / | 79.30 | 20.0 | *** METH DEFAULT *** |
| Q2 129.10 / | 39.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 2.000 / | 12503 |
| 2 | 5.000 / | 58013 |
| 3 | 7.490 / | 108458 |
| 4 | 9.990 / | 158435 |
| 5 | 19.998 / | 322167 |
| 6 | 39.960 / | 678496 |

Qualifier Peak Analysis ON
Curve Fit: Linear

3) Dodecanoic Acid

()

Ret. Time 7.735 min., Extract & Integrate from 7.235 to 8.235 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 60.00 | | | *** METH DEFAULT *** |
| Q1 73.10 | 91.40 | 20.0 | *** METH DEFAULT *** |
| Q2 129.10 | 30.90 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 1.990 / | 7296 |
| 2 | 4.990 / | 38633 |
| 3 | 7.480 / | 73334 |
| 4 | 9.970 / | 113308 |
| 5 | 19.950 / | 277225 |
| 6 | 39.900 / | 587121 |

Qualifier Peak Analysis ON
Curve Fit: Linear

4) Tetradecanoic Acid

()

1 2.000 / 1.98 on Data Page 1097
 2 4.940 / 4985
 3 7.410 / 13304
 4 9.880 / 20948
 5 19.760 / 98193
 6 39.530 / 245188

Qualifier Peak Analysis ON
 Curve Fit: Quadratic

8) Octadecanoic Acid

()

Ret. Time 15.219 min., Extract & Integrate from 14.719 to 15.719 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 60.00 | | | *** METH DEFAULT *** |
| Q1 73.00 | 97.20 | 20.0 | *** METH DEFAULT *** |
| Q2 129.10 | 45.70 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 1.980 / | 332 |
| 2 | 4.960 / | 2513 |
| 3 | 7.440 / | 8582 |
| 4 | 9.920 / | 13382 |
| 5 | 19.840 / | 49446 |
| 6 | 39.680 / | 146106 |

Qualifier Peak Analysis ON
 Curve Fit: Quadratic

9) Eicosanoic Acid

()

Ret. Time 18.626 min., Extract & Integrate from 18.126 to 19.126 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 60.00 | | | *** METH DEFAULT *** |
| Q1 73.00 | 109.60 | 20.0 | *** METH DEFAULT *** |
| Q2 129.00 | 47.20 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 2.000 / | -1 |
| 2 | 5.000 / | -1 |
| 3 | 7.490 / | -1 |
| 4 | 9.990 / | 1280 |
| 5 | 19.980 / | 6759 |
| 6 | 39.970 / | 30835 |

Qualifier Peak Analysis ON
 Curve Fit: Linear

10) MCHM (I)

()

Ret. Time 4.708 min., Extract & Integrate from 4.508 to 4.908 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 97.10 | 44.60 | 20.0 | *** METH DEFAULT *** |
| Q2 81.10 | 31.30 | 20.0 | *** METH DEFAULT *** |
| Q3 110.10 | 11.00 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 - | 1584 |
| 2 | 0.500 - | 4124 |
| 3 | 1.000 - | 9024 |
| 4 | 2.000 - | 18815 |
| 5 | 5.000 - | 50528 |
| 6 | 10.000 - | 106376 |

Qualifier Peak Analysis ON

Ret. Time 9.433 min., Extract & Integrate from 8.933 to 9.933 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 60.10 | | | *** METH DEFAULT *** |
| Q1 73.10 | 99.30 | 20.0 | *** METH DEFAULT *** |
| Q2 129.10 | 44.80 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 2.010 / | 2884 |
| 2 | 5.030 / | 19058 |
| 3 | 7.550 / | 44566 |
| 4 | 10.060 / | 73716 |
| 5 | 20.120 / | 197692 |
| 6 | 40.240 / | 445474 |

Qualifier Peak Analysis ON
Curve Fit: Linear

5) Hexadecanoic Acid ()

Ret. Time 11.971 min., Extract & Integrate from 11.471 to 12.471 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 73.10 | | | *** METH DEFAULT *** |
| Q1 60.00 | 92.00 | 20.0 | *** METH DEFAULT *** |
| Q2 129.10 | 41.00 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 2.010 / | 1345 |
| 2 | 5.030 / | 8062 |
| 3 | 7.540 / | 25617 |
| 4 | 10.050 / | 41500 |
| 5 | 20.100 / | 131503 |
| 6 | 40.200 / | 341157 |

Qualifier Peak Analysis ON
Curve Fit: Linear

6) Linoleic Acid ()

Ret. Time 14.699 min., Extract & Integrate from 14.499 to 14.899 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 67.10 | | | *** METH DEFAULT *** |
| Q1 81.10 | 80.80 | 20.0 | *** METH DEFAULT *** |
| Q2 95.10 | 62.70 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 1.980 / | -1 |
| 2 | 4.960 / | 2164 |
| 3 | 7.440 / | 6762 |
| 4 | 9.920 / | 12951 |
| 5 | 19.840 / | 69226 |
| 6 | 39.670 / | 236501 |

Qualifier Peak Analysis ON
Curve Fit: Quadratic

7) Oleic Acid ()

Ret. Time 14.803 min., Extract & Integrate from 14.603 to 15.003 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 69.10 | 55.80 | 20.0 | *** METH DEFAULT *** |
| Q2 83.10 | 43.70 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
|--------|----------|----------|

Curve Fit: Linear

11) MCHM (II)

()

Ret. Time 4.866 min., Extract & Integrate from 4.666 to 5.066 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 97.10 | 40.50 | 20.0 | *** METH DEFAULT *** |
| Q2 81.10 | 28.80 | 20.0 | *** METH DEFAULT *** |
| Q3 110.10 | 7.90 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 3114 |
| 2 | 0.500 ✓ | 8418 |
| 3 | 1.000 ✓ | 18888 |
| 4 | 2.000 ✓ | 39341 |
| 5 | 5.000 ✓ | 108963 |
| 6 | 10.000 ✓ | 212269 |

Qualifier Peak Analysis ON
Curve Fit: Linear

12) PPH

()

Ret. Time 5.921 min., Extract & Integrate from 5.421 to 6.421 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 94.10 | | | *** METH DEFAULT *** |
| Q1 152.10 | 17.80 | 20.0 | *** METH DEFAULT *** |
| Q2 108.10 | 16.30 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 4832 |
| 2 | 0.500 ✓ | 15514 |
| 3 | 1.000 ✓ | 36014 |
| 4 | 2.000 ✓ | 75438 |
| 5 | 5.000 ✓ | 191535 |
| 6 | 10.000 ✓ | 383473 |

Qualifier Peak Analysis ON
Curve Fit: Linear

13) 1,4-CHDM (I)

()

Ret. Time 6.522 min., Extract & Integrate from 6.322 to 6.722 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 95.10 | | | *** METH DEFAULT *** |
| Q1 67.10 | 37.10 | 20.0 | *** METH DEFAULT *** |
| Q2 108.10 | 15.50 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 1732 |
| 2 | 0.500 ✓ | 5607 |
| 3 | 1.000 ✓ | 14551 |
| 4 | 2.000 ✓ | 33100 |
| 5 | 5.000 ✓ | 85308 |
| 6 | 10.000 ✓ | 166492 |

Qualifier Peak Analysis ON
Curve Fit: Linear

14) 1,4-CHDM (II)

()

Ret. Time 6.626 min., Extract & Integrate from 6.426 to 6.826 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|--------|-----------|----------------|-------------|
|--------|-----------|----------------|-------------|

7-3614
(b) (7)
(C)

Tgt 95.10
Q1 67.10 64.50 20.0
Q2 108.10 15.00 20.0

*** METH DEFAULT ***
*** METH DEFAULT ***
*** METH DEFAULT ***

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | -1 |
| 2 | 0.500 ✓ | 2380 |
| 3 | 1.000 ✓ | 4788 |
| 4 | 2.000 ✓ | 10962 |
| 5 | 5.000 ✓ | 29286 |
| 6 | 10.000 ✓ | 59129 |

Qualifier Peak Analysis ON
Curve Fit: Linear

15) DMCH-1,4-DC

()

Ret. Time 7.040 min., Extract & Integrate from 6.540 to 7.540 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 81.10 | | | *** METH DEFAULT *** |
| Q1 108.10 | 50.80 | 20.0 | *** METH DEFAULT *** |
| Q2 140.10 | 75.00 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 3379 |
| 2 | 0.500 ✓ | 9528 |
| 3 | 1.000 ✓ | 21037 |
| 4 | 2.000 ✓ | 42484 |
| 5 | 5.000 ✓ | 108166 |
| 6 | 10.000 ✓ | 203191 |

Qualifier Peak Analysis ON
Curve Fit: Linear

16) Di-PPH (I)

()

Ret. Time 7.610 min., Extract & Integrate from 7.410 to 7.810 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 59.10 | | | *** METH DEFAULT *** |
| Q1 94.10 | 70.80 | 20.0 | *** METH DEFAULT *** |
| Q2 121.00 | 24.90 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 464 |
| 2 | 0.500 ✓ | 1824 |
| 3 | 1.000 ✓ | 4824 |
| 4 | 2.000 ✓ | 11307 |
| 5 | 5.000 ✓ | 36007 |
| 6 | 10.000 ✓ | 77931 |

Qualifier Peak Analysis ON
Curve Fit: Linear

17) di-PPH (II)

()

Ret. Time 7.731 min., Extract & Integrate from 7.531 to 7.931 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 94.10 | | | *** METH DEFAULT *** |
| Q1 103.10 | 101.20 | 20.0 | *** METH DEFAULT *** |
| Q2 210.20 | 39.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | 714 |
| 2 | 0.500 ✓ | 2288 |
| 3 | 1.000 ✓ | 4835 |
| 4 | 2.000 ✓ | 9848 |

7-31-14 (b) (7)

| | | |
|---|----------|-------|
| 5 | 5.000 ✓ | 26410 |
| 6 | 10.000 ✓ | 51800 |

Qualifier Peak Analysis ON
Curve Fit: Linear

18) di-PPH (III) ()

Ret. Time 7.807 min., Extract & Integrate from 7.607 to 8.007 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 94.00 | | | *** METH DEFAULT *** |
| Q1 103.00 | 110.30 | 20.0 | *** METH DEFAULT *** |
| Q2 210.20 | 39.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | -1 |
| 2 | 0.500 ✓ | -1 |
| 3 | 1.000 ✓ | 560 |
| 4 | 2.000 ✓ | 831 |
| 5 | 5.000 ✓ | 2299 |
| 6 | 10.000 ✓ | 5611 |

Qualifier Peak Analysis ON
Curve Fit: Linear

19) di-PPH (IV) ()

Ret. Time 7.862 min., Extract & Integrate from 7.662 to 8.062 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 94.00 | | | *** METH DEFAULT *** |
| Q1 103.10 | 126.20 | 20.0 | *** METH DEFAULT *** |
| Q2 210.10 | 28.30 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.200 ✓ | -1 |
| 2 | 0.500 ✓ | -1 |
| 3 | 1.000 ✓ | 308 |
| 4 | 2.000 ✓ | 562 |
| 5 | 5.000 ✓ | 1459 |
| 6 | 10.000 ✓ | 2695 |

Qualifier Peak Analysis ON
Curve Fit: Linear

20) Octanoic Acid-ME ()

Ret. Time 5.134 min., Extract & Integrate from 4.634 to 5.634 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 41.60 | 20.0 | *** METH DEFAULT *** |
| Q2 127.10 | 10.90 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 ✓ | 2746 |
| 2 | 0.190 ✓ | 6662 |
| 3 | 0.475 ✓ | 18127 |
| 4 | 0.950 ✓ | 37962 |
| 5 | 1.425 ✓ | 58363 |
| 6 | 2.850 ✓ | 116120 |

Qualifier Peak Analysis ON
Curve Fit: Linear

21) Decanoic Acid-ME ()

7-13-14 (b) (7)(C)

Ret. Time 6.344 min., Extract & Integrate from 5.844 to 6.844 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 54.50 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 18.10 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.160 / | 4628 |
| 2 | 0.320 / | 11101 |
| 3 | 0.800 / | 32072 |
| 4 | 1.600 / | 68466 |
| 5 | 2.400 / | 103405 |
| 6 | 4.800 / | 209319 |

Qualifier Peak Analysis ON
Curve Fit: Linear

22) Dodecanoic Acid-ME ()

Ret. Time 7.463 min., Extract & Integrate from 6.963 to 7.963 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 61.20 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 11.20 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.320 / | 10679 |
| 2 | 0.640 / | 25100 |
| 3 | 1.600 / | 67768 |
| 4 | 3.200 / | 138676 |
| 5 | 4.800 / | 208147 |
| 6 | 9.600 / | 391150 |

Qualifier Peak Analysis ON
Curve Fit: Linear

23) Tridecanoic Acid-ME ()

Ret. Time 8.168 min., Extract & Integrate from 7.668 to 8.668 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 63.90 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 13.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.160 / | 4376 |
| 2 | 0.320 / | 11087 |
| 3 | 0.800 / | 30997 |
| 4 | 1.600 / | 69449 |
| 5 | 2.400 / | 103213 |
| 6 | 4.800 / | 206449 |

Qualifier Peak Analysis ON
Curve Fit: Linear

24) Myristolic Acid-ME ()

Ret. Time 8.947 min., Extract & Integrate from 8.447 to 9.447 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 74.10 | 48.50 | 20.0 | *** METH DEFAULT *** |
| Q2 83.10 | 28.10 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 | 755 / |

1
2 0.190 / 2768
3 0.475 / 7438
4 0.950 / 18261
5 1.425 / 28820
6 2.850 / 60326

Qualifier Peak Analysis ON
Curve Fit: Linear

25) Tetradecanoic Acid-ME ()

Ret. Time 9.051 min., Extract & Integrate from 8.551 to 9.551 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 63.10 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 15.80 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.160 / | 3929 |
| 2 | 0.320 / | 9890 |
| 3 | 0.800 / | 31140 |
| 4 | 1.600 / | 69063 |
| 5 | 2.400 / | 104754 |
| 6 | 4.800 / | 211896 |

Qualifier Peak Analysis ON
Curve Fit: Linear

26) Pentadecanoic Acid-ME ()

Ret. Time 10.140 min., Extract & Integrate from 9.640 to 10.640 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 66.30 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 14.70 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 / | 1544 |
| 2 | 0.190 / | 4973 |
| 3 | 0.475 / | 17133 |
| 4 | 0.950 / | 38455 |
| 5 | 1.425 / | 61051 |
| 6 | 2.850 / | 125550 |

Qualifier Peak Analysis ON
Curve Fit: Linear

27) Palmitoleic Acid - ME *DO 7/25/14* ()

Ret. Time 11.167 min., Extract & Integrate from 10.667 to 11.667 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 69.10 | 56.50 | 20.0 | *** METH DEFAULT *** |
| Q2 74.10 | 51.50 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.320 / | 2096 |
| 2 | 0.640 / | 7475 |
| 3 | 1.600 / | 25979 |
| 4 | 3.200 / | 54646 |
| 5 | 4.800 / | 85282 |
| 6 | 9.600 / | 174274 |

Qualifier Peak Analysis ON
Curve Fit: Linear

7-34-14
(b) (7)
(C)

28) Hexadecanoic Acid-ME

()

Ret. Time 11.457 min., Extract & Integrate from 10.957 to 11.957 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 67.70 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 15.70 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.650 / | 15590 |
| 2 | 1.300 / | 43812 |
| 3 | 3.250 / | 147798 |
| 4 | 6.500 / | 277357 |
| 5 | 9.750 / | 418546 |
| 6 | 19.500 / | 817153 |

Qualifier Peak Analysis ON
Curve Fit: Linear

29) Heptadecanoic Acid-ME

()

Ret. Time 12.946 min., Extract & Integrate from 12.446 to 13.446 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 68.10 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 17.60 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.160 / | 1862 |
| 2 | 0.320 / | 7937 |
| 3 | 0.800 / | 32034 |
| 4 | 1.600 / | 64053 |
| 5 | 2.400 / | 99984 |
| 6 | 4.800 / | 207034 |

Qualifier Peak Analysis ON
Curve Fit: Linear

30) Linoleic Acid-ME

()

Ret. Time 14.057 min., Extract & Integrate from 13.857 to 14.257 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 67.10 | | | *** METH DEFAULT *** |
| Q1 81.10 | 81.90 | 20.0 | *** METH DEFAULT *** |
| Q2 95.10 | 59.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------------------------|----------|
| 1 | 0.650 0.670 / | 2760 |
| 2 | 1.300 1.328 / | 11912 |
| 3 | 3.250 3.20 / | 47002 |
| 4 | 6.500 6.400 / | 91893 |
| 5 | 9.750 9.600 / | 142337 |
| 6 | 19.500 19.200 / | 290518 |

Calibration curves for high concentration sets were compared and a 2% between the original curve and the second curve was observed. Therefore, the original concentration set was used.

(b) (7)(C)

8/6/14

7-31-14

(b) (7)(C)

Qualifier Peak Analysis ON
Curve Fit: Linear

31) Linolenic/Oleic Acid-MEs

()

Ret. Time 14.180 min., Extract & Integrate from 13.980 to 14.380 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 41.10 | 60.80 | 20.0 | *** METH DEFAULT *** |
| Q2 296.30 | 2.10 | 20.0 | *** METH DEFAULT *** |

(b) (7)(C)

Q3 292.30 0.60 20.0

*** METH DEFAULT ***

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 1.300 / | 11200 |
| 2 | 2.600 / | 31332 |
| 3 | 6.500 / | 100497 |
| 4 | 13.000 / | 193649 |
| 5 | 19.500 / | 283239 |
| 6 | 39.000 / | 544302 |

Qualifier Peak Analysis ON
Curve Fit: Linear

32) Elaidic Acid-ME ()

Ret. Time 14.273 min., Extract & Integrate from 14.073 to 14.473 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 69.10 | 51.10 | 20.0 | *** METH DEFAULT *** |
| Q2 83.10 | 47.10 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.130 / | 1382 |
| 2 | 0.260 / | 3563 |
| 3 | 0.650 / | 12251 |
| 4 | 1.300 / | 25930 |
| 5 | 1.950 / | 39015 |
| 6 | 3.900 / | 81076 |

Qualifier Peak Analysis ON
Curve Fit: Linear

33) Octadecanoic Acid-ME ()

Ret. Time 14.602 min., Extract & Integrate from 14.102 to 15.102 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 73.50 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 19.10 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.325 / | 6127 |
| 2 | 0.650 / | 19063 |
| 3 | 1.625 / | 71300 |
| 4 | 3.250 / | 134400 |
| 5 | 4.875 / | 206297 |
| 6 | 9.750 / | 407250 |

Qualifier Peak Analysis ON
Curve Fit: Linear

34) cis-11-Eicosanoic Acid-ME ()

Ret. Time 17.620 min., Extract & Integrate from 17.120 to 18.120 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 69.10 | 52.80 | 20.0 | *** METH DEFAULT *** |
| Q2 83.10 | 45.00 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 ✓ | -1 |
| 2 | 0.190 ✓ | 1539 |
| 3 | 0.475 ✓ | 7345 |
| 4 | 0.950 ✓ | 17178 |
| 5 | 1.425 ✓ | 30044 |
| 6 | 2.850 ✓ | 63310 |

(b) (7)
(C)7-31-14 (b) (7)
(C)

Qualifier Peak Analysis ON
Curve Fit: Linear

35) Eicosanoic Acid-ME ()

Ret. Time 18.043 min., Extract & Integrate from 17.543 to 18.543 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 74.50 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 19.80 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 / | 674 |
| 2 | 0.190 / | 3644 |
| 3 | 0.475 / | 16310 |
| 4 | 0.950 / | 33616 |
| 5 | 1.425 / | 55065 |
| 6 | 2.850 / | 115364 |

Qualifier Peak Analysis ON
Curve Fit: Linear

36) Erucic Acid-ME ()

Ret. Time 20.224 min., Extract & Integrate from 19.724 to 20.724 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 55.10 | | | *** METH DEFAULT *** |
| Q1 69.10 | 61.00 | 20.0 | *** METH DEFAULT *** |
| Q2 83.10 | 51.30 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 / | 302 |
| 2 | 0.190 / | 1147 |
| 3 | 0.475 / | 5449 |
| 4 | 0.950 / | 12151 |
| 5 | 1.425 / | 21890 |
| 6 | 2.850 / | 49848 |

Qualifier Peak Analysis ON
Curve Fit: Linear

37) Docosanoic Acid-ME ()

Ret. Time 20.511 min., Extract & Integrate from 20.011 to 21.011 min.

| Signal | Rel Resp. | Pct. Unc.(rel) | Integration |
|-----------|-----------|----------------|----------------------|
| Tgt 74.10 | | | *** METH DEFAULT *** |
| Q1 87.10 | 74.80 | 20.0 | *** METH DEFAULT *** |
| Q2 143.10 | 23.40 | 20.0 | *** METH DEFAULT *** |

| Lvl ID | Conc () | Response |
|--------|----------|----------|
| 1 | 0.095 / | 383 |
| 2 | 0.190 / | 1817 |
| 3 | 0.475 / | 11026 |
| 4 | 0.950 / | 25221 |
| 5 | 1.425 / | 42879 |
| 6 | 2.850 / | 96381 |

Qualifier Peak Analysis ON
Curve Fit: Linear

7-31-14

(b) (7)
(C)

END OF DATA ANALYSIS PARAMETERS

Thu Jun 26 13:42:02 2014

Method Path : C:\msdchem\1\METHODS\
 Method File (b) (7) RP1581_Fatty Acids.M
 Title : RP1581 (b) (7) Fatty Acids_&_MCHM
 Last Update : Thu Jun 19 16:20:55 2014
 Response Via : Initial Calibration

Calibration Files

1 =061814_003.D 2 =061814_004.D 3 =061814_005.D 4 =061814_006.D
 5 =061814_007.D 6 =061814_008.D

| Compound | 1 | 2 | 3 | 4 | 5 | 6 | Avg | %RSD |
|-----------------------|-------|-------|-------|-------|-------|-------|----------|-------|
| 1) Octanoic Acid | 0.852 | 1.449 | 1.787 | 1.876 | 2.175 | 2.297 | 1.739 E4 | 30.35 |
| 2) Decanoic Acid | 0.625 | 1.160 | 1.448 | 1.586 | 1.611 | 1.698 | 1.355 E4 | 29.82 |
| 3) Dodecanoic Acid | 0.367 | 0.774 | 0.980 | 1.136 | 1.390 | 1.471 | 1.020 E4 | 40.26 |
| 4) Tetradecanoic ... | 0.143 | 0.379 | 0.590 | 0.733 | 0.983 | 1.107 | 0.656 E4 | 55.39 |
| 5) Hexadecanoic Acid | 0.669 | 1.603 | 3.397 | 4.129 | 6.542 | 8.486 | 4.138 E3 | 71.44 |
| 6) Linoleic Acid | 0.436 | 0.909 | 1.306 | 3.489 | 5.962 | 2.420 | E3 | 95.00 |
| 7) Oleic Acid | 0.548 | 1.009 | 1.795 | 2.120 | 4.969 | 6.203 | 2.774 E3 | 82.24 |
| 8) Octadecanoic Acid | 0.168 | 0.507 | 1.153 | 1.349 | 2.492 | 3.682 | 1.559 E3 | 84.30 |
| 9) Eicosanoic Acid | | | 1.281 | 3.383 | 7.715 | 4.126 | E2 | 79.50 |
| 10) MCHM (I) | 0.792 | 0.825 | 0.902 | 0.941 | 1.011 | 1.064 | 0.922 E4 | 11.37 |
| 11) MCHM (II) | 1.557 | 1.684 | 1.889 | 1.967 | 2.179 | 2.123 | 1.900 E4 | 12.82 |
| 12) PPH | 2.416 | 3.103 | 3.601 | 3.772 | 3.831 | 3.835 | 3.426 E4 | 16.54 |
| 13) 1,4-CHDM (I) | 0.866 | 1.121 | 1.455 | 1.655 | 1.706 | 1.665 | 1.411 E4 | 24.42 |
| 14) 1,4-CHDM (II) | 4.760 | 4.788 | 5.481 | 5.857 | 5.913 | 5.360 | E3 | 10.45 |
| 15) DMCH-1,4-DC | 1.690 | 1.906 | 2.104 | 2.124 | 2.163 | 2.032 | 2.003 E4 | 8.91 |
| 16) Di-PPH (I) | 2.320 | 3.648 | 4.824 | 5.654 | 7.201 | 7.793 | 5.240 E3 | 39.82 |
| 17) di-PPH (II) | 3.570 | 4.576 | 4.835 | 4.924 | 5.282 | 5.180 | 4.728 E3 | 13.12 |
| 18) di-PPH (III) | | | 5.600 | 4.155 | 4.598 | 5.611 | 4.991 E2 | 14.67 |
| 19) di-PPH (IV) | | | 3.080 | 2.810 | 2.918 | 2.695 | 2.876 E2 | 5.70 |
| 20) Octanoic Acid-ME | 2.891 | 3.506 | 3.816 | 3.996 | 4.096 | 4.074 | 3.730 E4 | 12.49 |
| 21) Decanoic Acid-ME | 2.893 | 3.469 | 4.009 | 4.279 | 4.309 | 4.361 | 3.887 E4 | 15.15 |
| 22) Dodecanoic Aci... | 3.337 | 3.922 | 4.236 | 4.334 | 4.336 | 4.074 | 4.040 E4 | 9.40 |
| 23) Tridecanoic Ac... | 2.735 | 3.465 | 3.875 | 4.341 | 4.301 | 4.301 | 3.836 E4 | 16.64 |
| 24) Myristolic Aci... | 0.795 | 1.457 | 1.566 | 1.922 | 2.022 | 2.117 | 1.646 E4 | 29.83 |
| 25) Tetradecanoic ... | 2.456 | 3.091 | 3.893 | 4.316 | 4.365 | 4.415 | 3.756 E4 | 21.53 |
| 26) Pentadecanoic ... | 1.625 | 2.617 | 3.607 | 4.048 | 4.284 | 4.405 | 3.431 E4 | 31.96 |
| 27) Palmitoleic Acid | 0.655 | 1.168 | 1.624 | 1.708 | 1.777 | 1.815 | 1.458 E4 | 31.41 |
| 28) Hexadecanoic A... | 2.398 | 3.370 | 4.548 | 4.267 | 4.293 | 4.191 | 3.844 E4 | 21.16 |
| 29) Heptadecanoic ... | 1.164 | 2.480 | 4.004 | 4.003 | 4.166 | 4.313 | 3.355 E4 | 37.66 |
| 30) Linoleic Acid-ME | 0.425 | 0.916 | 1.446 | 1.414 | 1.460 | 1.490 | 1.192 E4 | 36.37 |
| 31) Linolenic/Olei... | 0.862 | 1.205 | 1.546 | 1.490 | 1.453 | 1.396 | 1.325 E4 | 19.28 |
| 32) Elaidic Acid-ME | 1.063 | 1.370 | 1.885 | 1.995 | 2.001 | 2.079 | 1.732 E4 | 23.99 |
| 33) Octadecanoic A... | 1.885 | 2.933 | 4.388 | 4.135 | 4.232 | 4.177 | 3.625 E4 | 27.64 |
| 34) cis-11-Eicosan... | 0.810 | 1.546 | 1.808 | 2.108 | 2.221 | 1.699 | E4 | 33.12 |
| 35) Eicosanoic Aci... | 0.709 | 1.918 | 3.434 | 3.539 | 3.864 | 4.048 | 2.919 E4 | 45.20 |
| 36) Erucic Acid-ME | 0.318 | 0.604 | 1.147 | 1.279 | 1.536 | 1.749 | 1.105 E4 | 49.60 |
| 37) Docosanoic Aci... | 0.403 | 0.956 | 2.321 | 2.655 | 3.009 | 3.382 | 2.121 E4 | 55.83 |

(#) = Out of Range

(b) (7) RP1581_Fatty Acids.M Mon Jun 23 10:40:09 2014
 (C)

Method Path : C:\msdchem\1\METHODS\
 Method File (b) (7) RP1581_Fatty Acids.M
 Title : RP1581 (b) (7) Fatty Acids_&_MCHM
 Last Update : Thu Jun 19 16:20:55 2014
 Response Via : Initial Calibration

Calibration Files

1 =061814_003 2 =061814_004 3 =061814_005 4 =061814_006
 5 =061814_007 6 =061814_008

| | Compound | Fit | Constant | Linear | Quad | RSD/Cf |
|-----|---------------------|------|------------|-----------|-----------|--------|
| 1) | Octanoic Acid | Lin | -4.3900 e4 | 2.3992 e4 | ----- | 0.9995 |
| 2) | Decanoic Acid | Lin | -2.3998 e4 | 1.7552 e4 | ----- | 0.9996 |
| 3) | Dodecanoic Acid | Lin | -3.6088 e4 | 1.5584 e4 | ----- | 0.9989 |
| 4) | Tetradecanoic Acid | Lin | -3.8017 e4 | 1.1899 e4 | ----- | 0.9969 |
| 5) | Hexadecanoic Acid | Lin | -3.8568 e4 | 9.1910 e3 | ----- | 0.9888 |
| 6) | Linoleic Acid | Quad | -1.1540 e4 | 1.6843 e3 | 1.1534 e2 | 0.9994 |
| 7) | Oleic Acid | Quad | -1.4862 e4 | 3.9178 e3 | 6.8260 e1 | 0.9944 |
| 8) | Octadecanoic Acid | Quad | -5.0032 e3 | 1.4694 e3 | 5.9157 e1 | 0.9991 |
| 9) | Eicosanoic Acid | Lin | -1.0753 e4 | 1.0171 e3 | ----- | 0.9752 |
| 10) | MCHM (I) | Lin | -1.6659 e3 | 1.0719 e4 | ----- | 0.9994 |
| 11) | MCHM (II) | Lin | -1.9784 e3 | 2.1544 e4 | ----- | 0.9995 |
| 12) | PPH | Lin | -2.7455 e3 | 3.8678 e4 | ----- | 1.0000 |
| 13) | 1,4-CHDM (I) | Lin | -1.6377 e3 | 1.6931 e4 | ----- | 0.9995 |
| 14) | 1,4-CHDM (II) | Lin | -9.2725 e2 | 6.0098 e3 | ----- | 0.9999 |
| 15) | DMCH-1,4-DC | Lin | 7.6438 e2 | 2.0492 e4 | ----- | 0.9988 |
| 16) | Di-PPH (I) | Lin | -2.8396 e3 | 7.9890 e3 | ----- | 0.9981 |
| 17) | di-PPH (II) | Lin | -3.3461 e2 | 5.2354 e3 | ----- | 0.9998 |
| 18) | di-PPH (III) | Lin | -2.4365 e2 | 5.7087 e2 | ----- | 0.9890 |
| 19) | di-PPH (IV) | Lin | 5.5786 e1 | 2.6671 e2 | ----- | 0.9981 |
| 20) | Octanoic Acid-ME | Lin | -1.1467 e3 | 4.1246 e4 | ----- | 0.9999 |
| 21) | Decanoic Acid-ME | Lin | -2.7727 e3 | 4.4209 e4 | ----- | 1.0000 |
| 22) | Dodecanoic Acid-ME | Lin | 2.1306 e3 | 4.1108 e4 | ----- | 0.9984 |
| 23) | Tridecanoic Acid-ME | Lin | -2.4776 e3 | 4.3694 e4 | ----- | 0.9997 |
| 24) | Myristolic Acid-ME | Lin | -1.9497 e3 | 2.1732 e4 | ----- | 0.9992 |
| 25) | Tetradecanoic Ac... | Lin | -3.8739 e3 | 4.5031 e4 | ----- | 0.9999 |
| 26) | Pentadecanoic Ac... | Lin | -3.7080 e3 | 4.5272 e4 | ----- | 0.9998 |
| 27) | Palmitoleic Acid-ME | Lin | -4.1322 e3 | 1.8579 e4 | ----- | 1.0000 |
| 28) | Hexadecanoic Aci... | Lin | -2.4762 e3 | 4.2372 e4 | ----- | 0.9990 |
| 29) | Heptadecanoic Ac... | Lin | -5.3766 e3 | 4.4163 e4 | ----- | 0.9998 |
| 30) | Linoleic Acid-ME | Lin | -6.1783 e3 | 1.5226 e4 | ----- | 0.9997 |
| 31) | Linolenic/Oleic ... | Lin | 1.7957 e3 | 1.4084 e4 | ----- | 0.9982 |
| 32) | Elaidic Acid-ME | Lin | -1.6839 e3 | 2.1162 e4 | ----- | 0.9999 |
| 33) | Octadecanoic Aci... | Lin | -4.1573 e3 | 4.2461 e4 | ----- | 0.9992 |
| 34) | cis-11-Eicosanoi... | Lin | -3.7378 e3 | 2.3447 e4 | ----- | 0.9989 |
| 35) | Eicosanoic Acid-ME | Lin | -4.1918 e3 | 4.1742 e4 | ----- | 0.9995 |
| 36) | Erucic Acid-ME | Lin | -2.9475 e3 | 1.8124 e4 | ----- | 0.9946 |
| 37) | Docosanoic Acid-ME | Lin | -5.4125 e3 | 3.5118 e4 | ----- | 0.9970 |

(b) (7) (C) RP1581_Fatty Acids.M Mon Jun 23 10:38:54 2014

Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
 Data File : 061814_003.D
 Acq On : 18 Jun 2014 9:37 pm
 Operator : (b) (7)(C)
 Sample : Std Level 1-A
 Misc : Calibration Standard 1
 ALS Vial : 3 Sample Multiplier: 1

Quant Time: Jun 19 16:02:27 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration

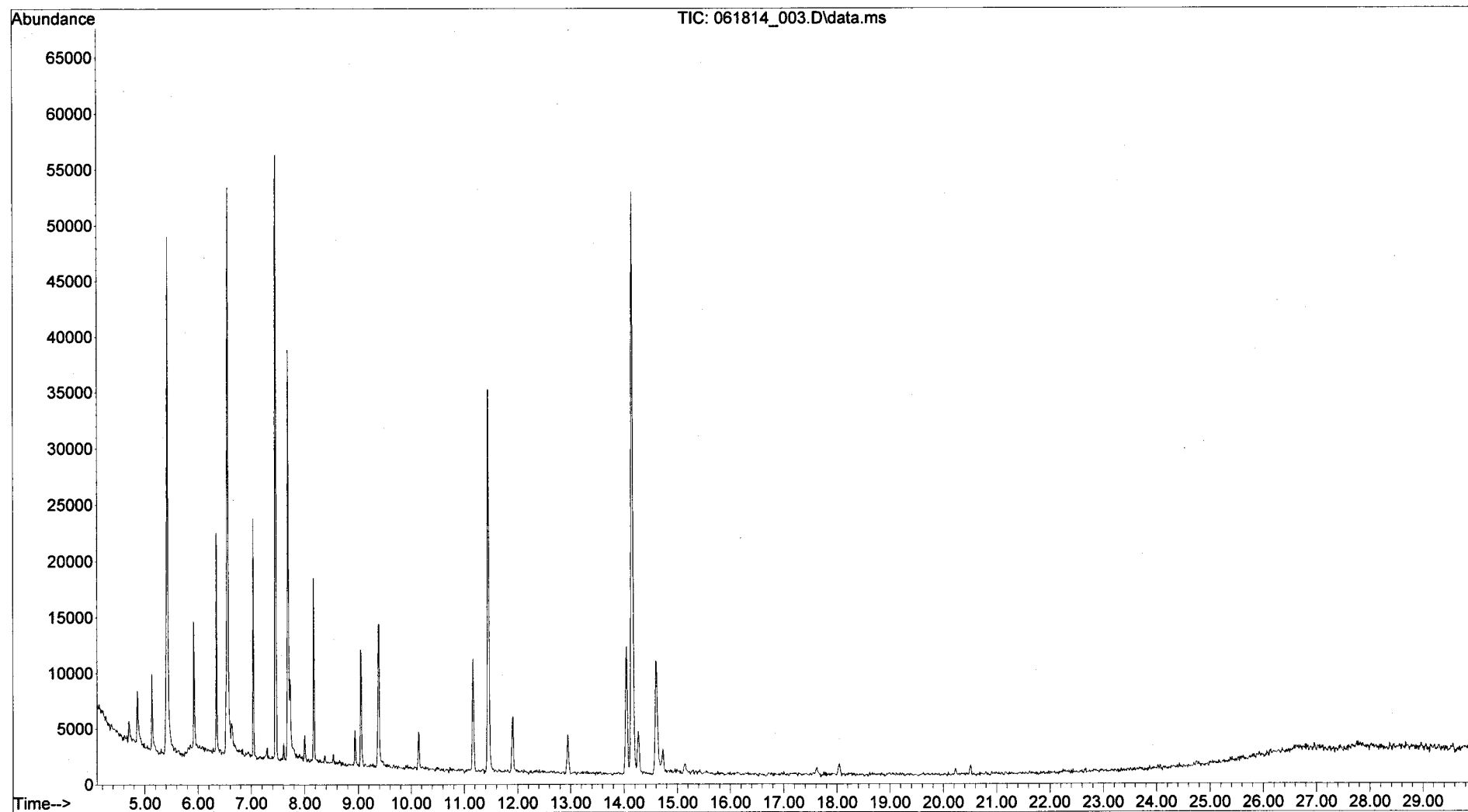
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) | |
|---|--------|------|----------|------|-------|-----------|--------|
| Target Compounds | | | | | | | Qvalue |
| 1) Octanoic Acid | 5.434 | 60 | 17126 | No | Calib | | |
| 2) Decanoic Acid | 6.564 | 60 | 12503 | No | Calib | | |
| 3) Dodecanoic Acid | 7.693 | 60 | 7296 | No | Calib | | |
| 4) Tetradecanoic Acid | 9.393 | 60 | 2884 | No | Calib | # | |
| 5) Hexadecanoic Acid | 11.911 | 73 | 1345 | No | Calib | # | |
| 6) Linoleic Acid | 0.000 | | 0 | N.D. | d | | |
| 7) Oleic Acid | 14.730 | 55 | 1097 | No | Calib | | |
| 8) Octadecanoic Acid | 15.144 | 60 | 332 | No | Calib | # | |
| 9) Eicosanoic Acid | 0.000 | | 0 | N.D. | | | |
| 10) MCHM (I) | 4.698 | 55 | 1584 | No | Calib | # | |
| 11) MCHM (II) | 4.864 | 55 | 3114 | No | Calib | # | |
| 12) PPH | 5.921 | 94 | 4832 | No | Calib | | |
| 13) 1,4-CHDM (I) | 6.522 | 95 | 1732 | No | Calib | | |
| 14) 1,4-CHDM (II) | 0.000 | | 0 | N.D. | d | | |
| 15) DMCH-1,4-DC | 7.040 | 81 | 3379 | No | Calib | | |
| 16) Di-PPH (I) | 7.610 | 59 | 464 | No | Calib | | |
| 17) di-PPH (II) | 7.724 | 94 | 714 | No | Calib | # | |
| 18) di-PPH (III) | 0.000 | | 0 | N.D. | d | | |
| 19) di-PPH (IV) | 0.000 | | 0 | N.D. | d | | |
| 20) Octanoic Acid-ME | 5.133 | 74 | 2746 | No | Calib | | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 4628 | No | Calib | | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 10679 | No | Calib | | |
| 23) Tridecanoic Acid-ME | 8.170 | 74 | 4376 | No | Calib | # | |
| 24) Myristolic Acid-ME | 8.937 | 55 | 755 | No | Calib | | |
| 25) Tetradecanoic Acid-ME | 9.051 | 74 | 3929 | No | Calib | | |
| 26) Pentadecanoic Acid-ME | 10.139 | 74 | 1544 | No | Calib | # | |
| 27) Palmitoleic Acid - ME ^{DU} 7/25/14 | 11.165 | 55 | 2096 | No | Calib | | |
| 28) Hexadecanoic Acid-ME | 11.455 | 74 | 15590 | No | Calib | | |
| 29) Heptadecanoic Acid-ME | 12.947 | 74 | 1862 | No | Calib | # | |
| 30) Linoleic Acid-ME | 14.046 | 67 | 2760 | No | Calib | | |
| 31) Linolenic/Oleic Acid-MES | 14.149 | 55 | 11200 | No | Calib | # | |
| 32) Elaidic Acid-ME | 14.263 | 55 | 1382 | No | Calib | | |
| 33) Octadecanoic Acid-ME | 14.595 | 74 | 6127 | No | Calib | | |
| 34) cis-11-Eicosanoic Acid-ME | 0.000 | | 0 | N.D. | d | | |
| 35) Eicosanoic Acid-ME | 18.046 | 74 | 674 | No | Calib | # | |
| 36) Erucic Acid-ME | 20.222 | 55 | 302 | No | Calib | # | |
| 37) Docosanoic Acid-ME | 20.512 | 74 | 383 | No | Calib | # | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581(b) (7) 061314\DBH_061814 Run\
 Data File : 061814_003.D
 Acq On : 18 Jun 2014 9:37 pm
 Operator : (b) (7)(C)
 Sample : Std Level 1-A
 Misc : Calibration Standard 1
 ALS Vial : 3 Sample Multiplier: 1

Quant Time: Jun 19 16:02:27 2014
 Quant Method : C:\msdchem\1\METHODS(b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581(b) (7) Fatty Acids (C) MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



Data Path : D:\RP1581\ (b) (7) 061314 (b) (7) 061814 Run\
Data File : 061814_004.D
Acq On : 18 Jun 2014 10:12 pm
Operator : (b) (7)
Sample : (b) (7) Std Level 2-A
Misc : Calibration Standard 2
ALS Vial : 4 Sample Multiplier: 1

Quant Time: Jun 19 16:04:14 2014

Quant Method : C:\msdchem\1\METHODS\ (b) (7) RP1581_Fatty Acids.M

Quant Title : RP1581_DBH_Fatty Acids & MCHM

QLast Update : Thu Jun 19 10:44:37 2014

Response via : Initial Calibration

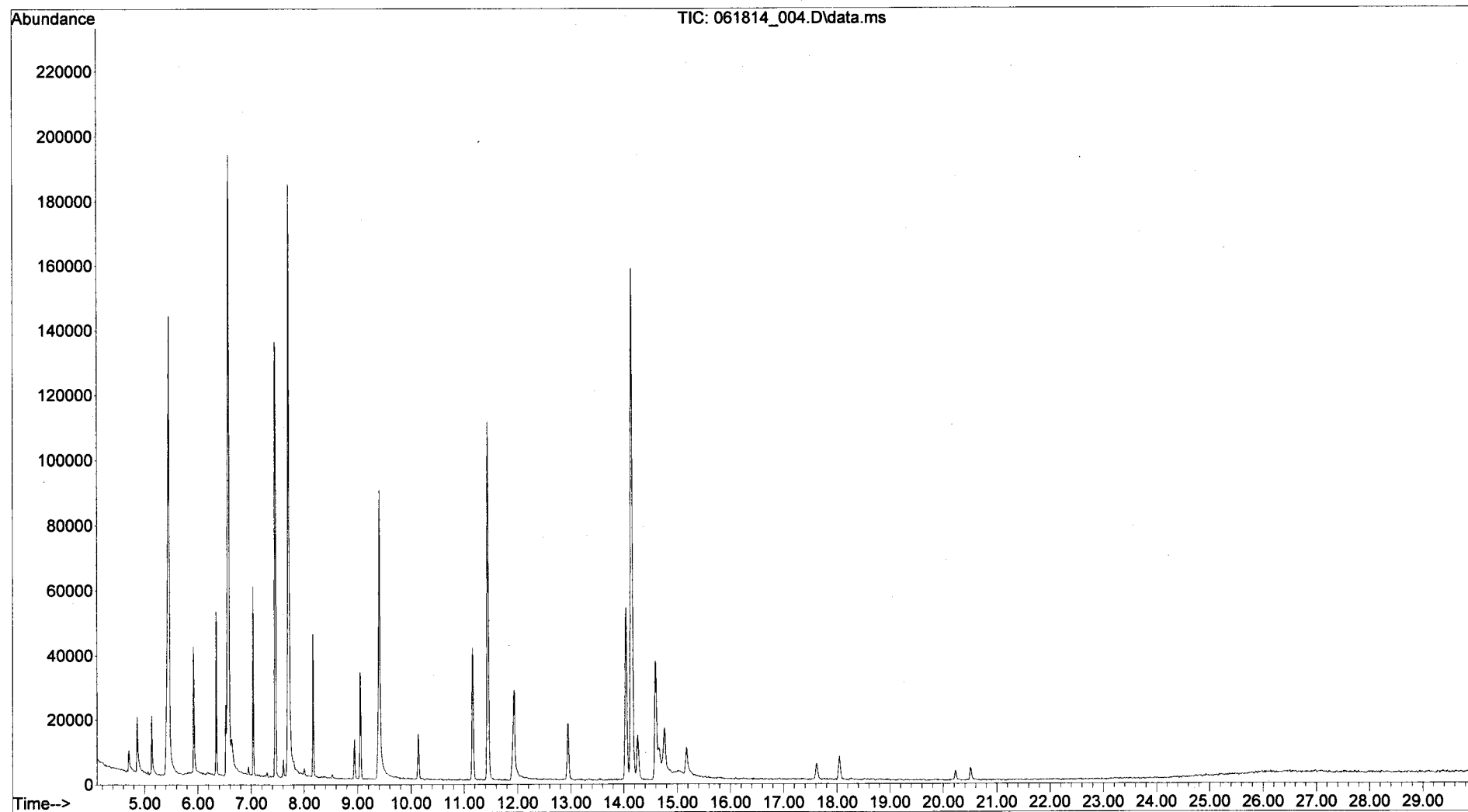
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) |
|---|--------|------|----------|------|-------|-----------|
| ----- | | | | | | |
| Target Compounds | | | | | | Qvalue |
| 1) Octanoic Acid | 5.465 | 60 | 72752 | No | Calib | |
| 2) Decanoic Acid | 6.584 | 60 | 58013 | No | Calib | |
| 3) Dodecanoic Acid | 7.714 | 60 | 38633 | No | Calib | |
| 4) Tetradecanoic Acid | 9.413 | 60 | 19058 | No | Calib | |
| 5) Hexadecanoic Acid | 11.942 | 73 | 8062 | No | Calib | |
| 6) Linoleic Acid | 14.657 | 67 | 2164 | No | Calib | |
| 7) Oleic Acid | 14.761 | 55 | 4985 | No | Calib | |
| 8) Octadecanoic Acid | 15.175 | 60 | 2513 | No | Calib | |
| 9) Eicosanoic Acid | 0.000 | | 0 | N.D. | d | |
| 10) MCHM (I) | 4.709 | 55 | 4124 | No | Calib | # |
| 11) MCHM (II) | 4.864 | 55 | 8418 | No | Calib | |
| 12) PPH | 5.921 | 94 | 15514 | No | Calib | |
| 13) 1,4-CHDM (I) | 6.522 | 95 | 5607 | No | Calib | |
| 14) 1,4-CHDM (II) | 6.636 | 95 | 2380 | No | Calib | # |
| 15) DMCH-1,4-DC | 7.040 | 81 | 9528 | No | Calib | |
| 16) Di-PPH (I) | 7.610 | 59 | 1824 | No | Calib | |
| 17) di-PPH (II) | 7.724 | 94 | 2288 | No | Calib | |
| 18) di-PPH (III) | 0.000 | | 0 | N.D. | d | |
| 19) di-PPH (IV) | 0.000 | | 0 | N.D. | d | |
| 20) Octanoic Acid-ME | 5.133 | 74 | 6662 | No | Calib | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 11101 | No | Calib | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 25100 | No | Calib | |
| 23) Tridecanoic Acid-ME | 8.170 | 74 | 11087 | No | Calib | |
| 24) Myristolic Acid-ME | 8.947 | 55 | 2768 | No | Calib | # |
| 25) Tetradecanoic Acid-ME | 9.051 | 74 | 9890 | No | Calib | |
| 26) Pentadecanoic Acid-ME | 10.139 | 74 | 4973 | No | Calib | |
| 27) Palmitoleic Acid - ME ^{pu} 7/25/14 | 11.165 | 55 | 7475 | No | Calib | |
| 28) Hexadecanoic Acid-ME | 11.445 | 74 | 43812 | No | Calib | |
| 29) Heptadecanoic Acid-ME | 12.947 | 74 | 7937 | No | Calib | |
| 30) Linoleic Acid-ME | 14.046 | 67 | 11912 | No | Calib | |
| 31) Linolenic/Oleic Acid-MEs | 14.149 | 55 | 31332 | No | Calib | # |
| 32) Elaidic Acid-ME | 14.263 | 55 | 3563 | No | Calib | |
| 33) Octadecanoic Acid-ME | 14.595 | 74 | 19063 | No | Calib | |
| 34) cis-11-Eicosanoic Acid-ME | 17.621 | 55 | 1539 | No | Calib | |
| 35) Eicosanoic Acid-ME | 18.035 | 74 | 3644 | No | Calib | |
| 36) Erucic Acid-ME | 20.222 | 55 | 1147 | No | Calib | # |
| 37) Docosanoic Acid-ME | 20.502 | 74 | 1817 | No | Calib | # |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581\ (b) (7) 061314\ (b) (7) 061814 Run\
 Data File : 061814_004 (C)
 Acq On : 18 Jun 2014 10:12 pm
 Operator : (b) (7)
 Sample : (b) (7) Level 2-A
 Misc : Calibration Standard 2
 ALS Vial : 4 Sample Multiplier: 1

Quant Time: Jun 19 16:04:14 2014
 Quant Method : C:\msdchem\1\METHODS\DBH_RP1581_Fatty Acids.M
 Quant Title : RP1581_ (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



Quantitation Report

(QT Reviewed)

Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
 Data File : 061814_00 (C)
 Acq On : 18 Jun 2014 10:48 pm
 Operator : (b) (7)(C)
 Sample : Std Level 3-A
 Misc : Calibration Standard 3
 ALS Vial : 5 Sample Multiplier: 1

Quant Time: Jun 19 16:09:36 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Aci (C) MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration

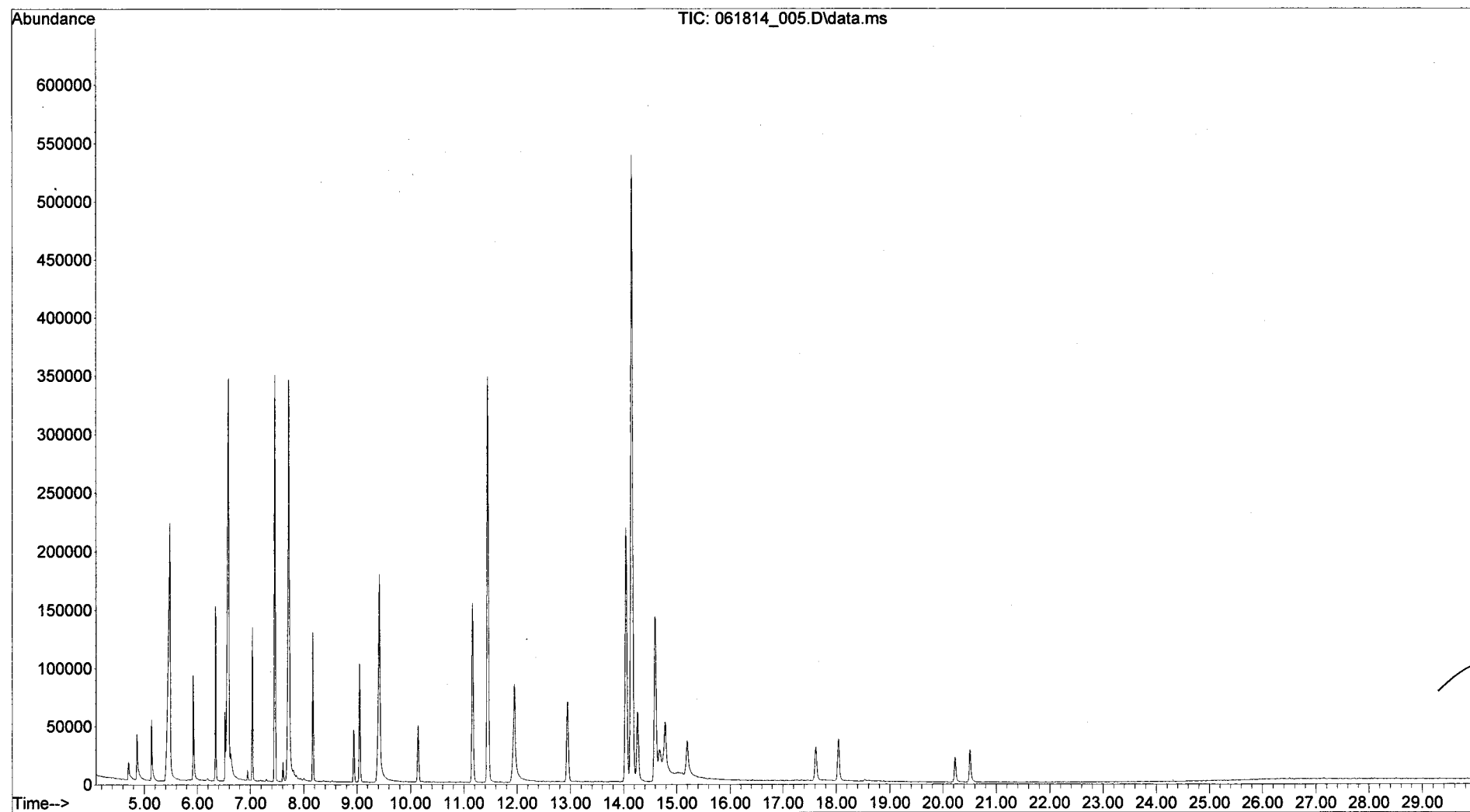
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) | |
|--|--------|------|----------|------|-------|-----------|--------|
| ----- | | | | | | | |
| Target Compounds | | | | | | | Qvalue |
| 1) Octanoic Acid | 5.486 | 60 | 134541 | No | Calib | | |
| 2) Decanoic Acid | 6.595 | 60 | 108458 | No | Calib | | |
| 3) Dodecanoic Acid | 7.724 | 60 | 73334 | No | Calib | | |
| 4) Tetradecanoic Acid | 9.424 | 60 | 44566 | No | Calib | | |
| 5) Hexadecanoic Acid | 11.952 | 73 | 25617 | No | Calib | | |
| 6) Linoleic Acid | 14.678 | 67 | 6762 | No | Calib | | |
| 7) Oleic Acid | 14.781 | 55 | 13304 | No | Calib | | |
| 8) Octadecanoic Acid | 15.196 | 60 | 8582 | No | Calib | | |
| 9) Eicosanoic Acid | 0.000 | | 0 | N.D. | d | | |
| 10) MCHM (I) | 4.709 | 55 | 9024 | No | Calib | | # |
| 11) MCHM (II) | 4.864 | 55 | 18888 | No | Calib | | |
| 12) PPH | 5.921 | 94 | 36014 | No | Calib | | |
| 13) 1,4-CHDM (I) | 6.522 | 95 | 14551 | No | Calib | | |
| 14) 1,4-CHDM (II) | 6.636 | 95 | 4788 | No | Calib | | |
| 15) DMCH-1,4-DC | 7.040 | 81 | 21037 | No | Calib | | |
| 16) Di-PPH (I) | 7.610 | 59 | 4824 | No | Calib | | |
| 17) di-PPH (II) | 7.735 | 94 | 4835 | No | Calib | | |
| 18) di-PPH (III) | 7.807 | 94 | 560 | No | Calib | | |
| 19) di-PPH (IV) | 7.859 | 94 | 308 | No | Calib | | # |
| 20) Octanoic Acid-ME | 5.133 | 74 | 18127 | No | Calib | | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 32072 | No | Calib | | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 67768 | No | Calib | | |
| 23) Tridecanoic Acid-ME | 8.170 | 74 | 30997 | No | Calib | | |
| 24) Myristolic Acid-ME | 8.937 | 55 | 7438 | No | Calib | | |
| 25) Tetradecanoic Acid-ME | 9.051 | 74 | 31140 | No | Calib | | |
| 26) Pentadecanoic Acid-ME | 10.139 | 74 | 17133 | No | Calib | | |
| 27) Palmitoleic Acid - ME <i>DA, 7/25/14</i> | 11.165 | 55 | 25979 | No | Calib | | |
| 28) Hexadecanoic Acid-ME | 11.455 | 74 | 147798 | No | Calib | | |
| 29) Heptadecanoic Acid-ME | 12.947 | 74 | 32034 | No | Calib | | |
| 30) Linoleic Acid-ME | 14.046 | 67 | 47002 | No | Calib | | |
| 31) Linolenic/Oleic Acid-MES | 14.160 | 55 | 100497 | No | Calib | | |
| 32) Elaidic Acid-ME | 14.263 | 55 | 12251 | No | Calib | | |
| 33) Octadecanoic Acid-ME | 14.595 | 74 | 71300 | No | Calib | | |
| 34) cis-11-Eicosanoic Acid-ME | 17.611 | 55 | 7345 | No | Calib | | |
| 35) Eicosanoic Acid-ME | 18.046 | 74 | 16310 | No | Calib | | |
| 36) Erucic Acid-ME | 20.232 | 55 | 5449 | No | Calib | | |
| 37) Docosanoic Acid-ME | 20.512 | 74 | 11026 | No | Calib | | |
| ----- | | | | | | | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581\ (b) (7) 061314\ (b) (7) 061814 Run\
 Data File : 061814_005.D (b) (7)
 Acq On : 18 Jun 2014 10:48 pm
 Operator : (b) (7)
 Sample : Std Level 3-A
 Misc : Calibration Standard 3
 ALS Vial : 5 Sample Multiplier: 1

Quant Time: Jun 19 16:09:36 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
 Data File : 061814_006.D (b) (7) (C)
 Acq On : 18 Jun 2014 11:24 pm
 Operator : (b) (7)
 Sample : Std Level 4-A
 Misc : Calibration Standard 4
 ALS Vial : 6 Sample Multiplier: 1

Quant Time: Jun 19 16:08:47 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration

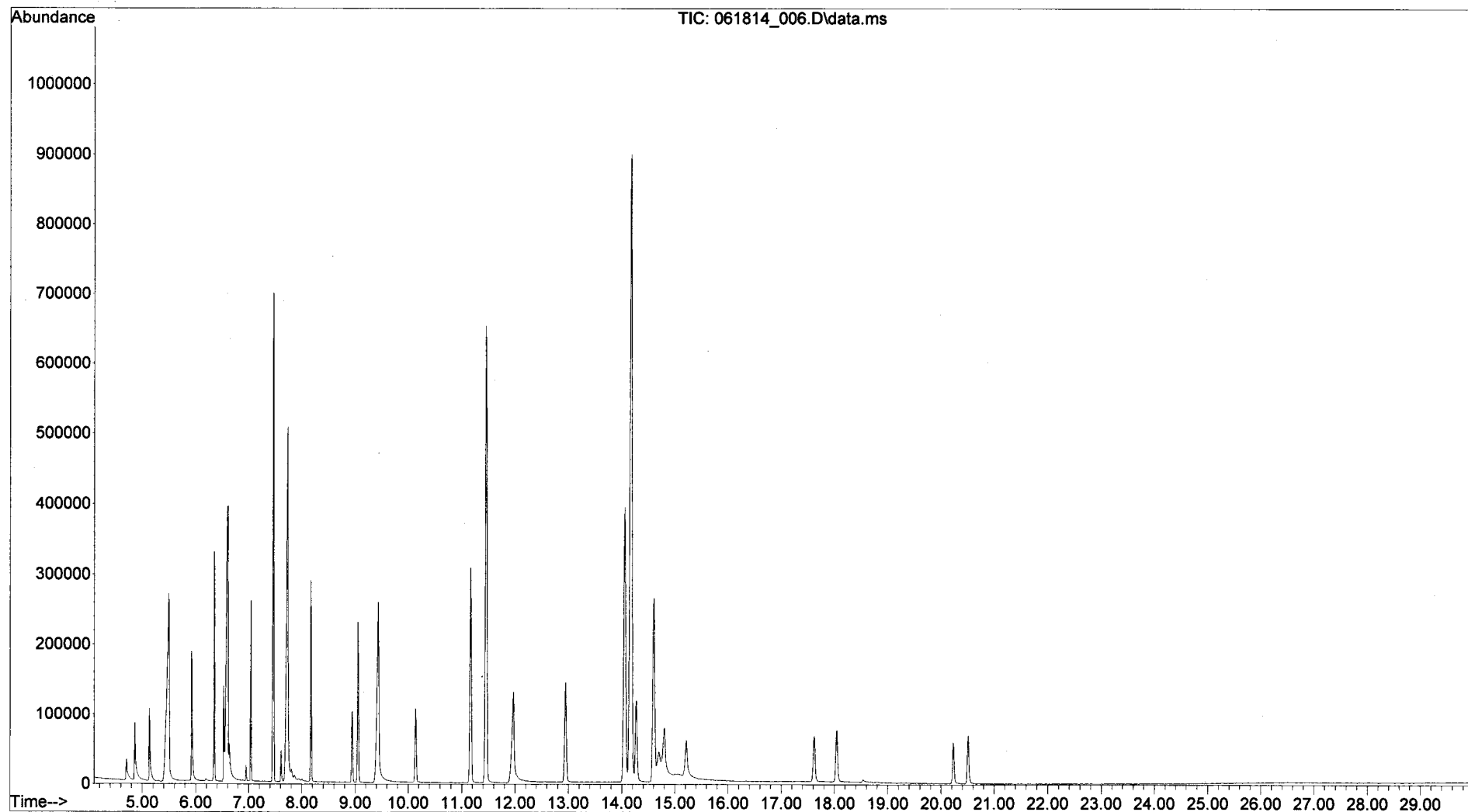
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) | |
|-------------------------------|--------|------|----------|------|-------|-----------|--------|
| ----- | | | | | | | |
| Target Compounds | | | | | | | Qvalue |
| 1) Octanoic Acid | 5.496 | 60 | 188369 | No | Calib | | |
| 2) Decanoic Acid | 6.595 | 60 | 158435 | No | Calib | | |
| 3) Dodecanoic Acid | 7.734 | 60 | 113308 | No | Calib | | |
| 4) Tetradecanoic Acid | 9.434 | 60 | 73716 | No | Calib | | |
| 5) Hexadecanoic Acid | 11.973 | 73 | 41500 | No | Calib | | |
| 6) Linoleic Acid | 14.698 | 67 | 12951 | No | Calib | | |
| 7) Oleic Acid | 14.802 | 55 | 20948 | No | Calib | | |
| 8) Octadecanoic Acid | 15.217 | 60 | 13382 | No | Calib | | |
| 9) Eicosanoic Acid | 18.543 | 60 | 1280 | No | Calib | | |
| 10) MCHM (I) | 4.708 | 55 | 18815 | No | Calib | | |
| 11) MCHM (II) | 4.864 | 55 | 39341 | No | Calib | | |
| 12) PPH | 5.921 | 94 | 75438 | No | Calib | | |
| 13) 1,4-CHDM (I) | 6.522 | 95 | 33100 | No | Calib | | |
| 14) 1,4-CHDM (II) | 6.626 | 95 | 10962 | No | Calib | | |
| 15) DMCH-1,4-DC | 7.040 | 81 | 42484 | No | Calib | | |
| 16) Di-PPH (I) | 7.610 | 59 | 11307 | No | Calib | | |
| 17) di-PPH (II) | 7.734 | 94 | 9848 | No | Calib | | |
| 18) di-PPH (III) | 7.807 | 94 | 831 | No | Calib | | |
| 19) di-PPH (IV) | 7.859 | 94 | 562 | No | Calib | | |
| 20) Octanoic Acid-ME | 5.133 | 74 | 37962 | No | Calib | | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 68466 | No | Calib | | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 138676 | No | Calib | | |
| 23) Tridecanoic Acid-ME | 8.170 | 74 | 69449 | No | Calib | | |
| 24) Myristolic Acid-ME | 8.937 | 55 | 18261 | No | Calib | | |
| 25) Tetradecanoic Acid-ME | 9.051 | 74 | 69063 | No | Calib | | |
| 26) Pentadecanoic Acid-ME | 10.139 | 74 | 38455 | No | Calib | | |
| 27) Palmitoleic Acid-ME | 11.165 | 55 | 54646 | No | Calib | | |
| 28) Hexadecanoic Acid-ME | 11.455 | 74 | 277357 | No | Calib | | |
| 29) Heptadecanoic Acid-ME | 12.947 | 74 | 64053 | No | Calib | | |
| 30) Linoleic Acid-ME | 14.056 | 67 | 91893 | No | Calib | | |
| 31) Linolenic/Oleic Acid-MES | 14.180 | 55 | 193649 | No | Calib | | |
| 32) Elaidic Acid-ME | 14.274 | 55 | 25930 | No | Calib | | |
| 33) Octadecanoic Acid-ME | 14.605 | 74 | 134400 | No | Calib | | |
| 34) cis-11-Eicosanoic Acid-ME | 17.621 | 55 | 17178 | No | Calib | | |
| 35) Eicosanoic Acid-ME | 18.046 | 74 | 33616 | No | Calib | | |
| 36) Erucic Acid-ME | 20.222 | 55 | 12151 | No | Calib | | |
| 37) Docosanoic Acid-ME | 20.512 | 74 | 25221 | No | Calib | | |
| ----- | | | | | | | |

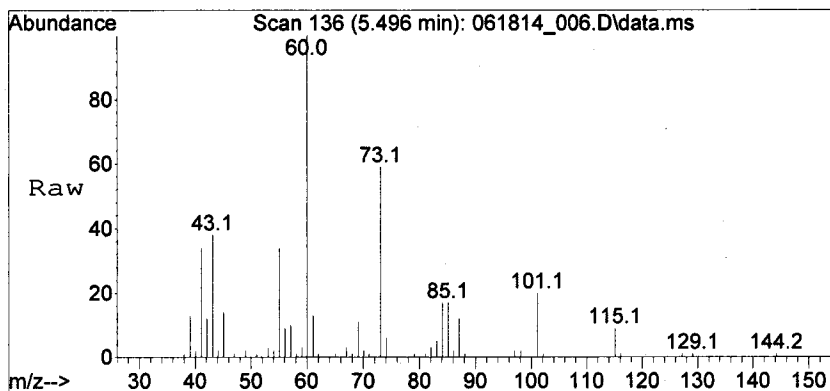
(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581 (b) (7) 061314\ (b) (7) 061814 Run\
 Data File : 061814_006.D
 Acq On : 18 Jun 2014 11:24 pm
 Operator : (b) (7)
 Sample : (b) (7) Std Level 4-A
 Misc : Calibration Standard 4
 ALS Vial : 6 Sample Multiplier: 1

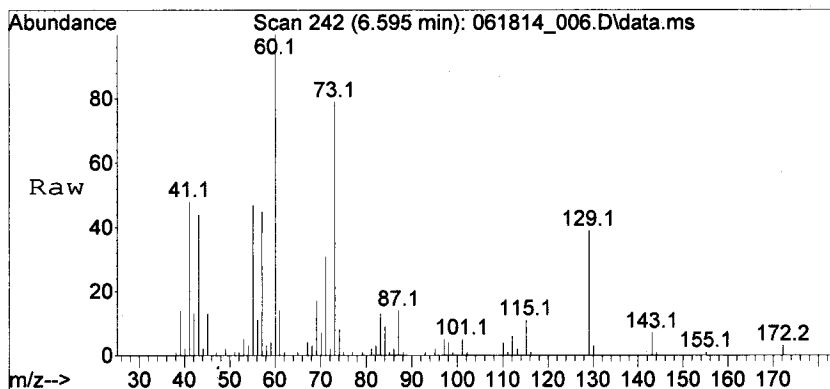
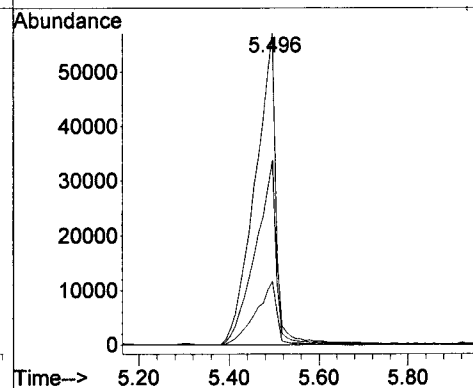
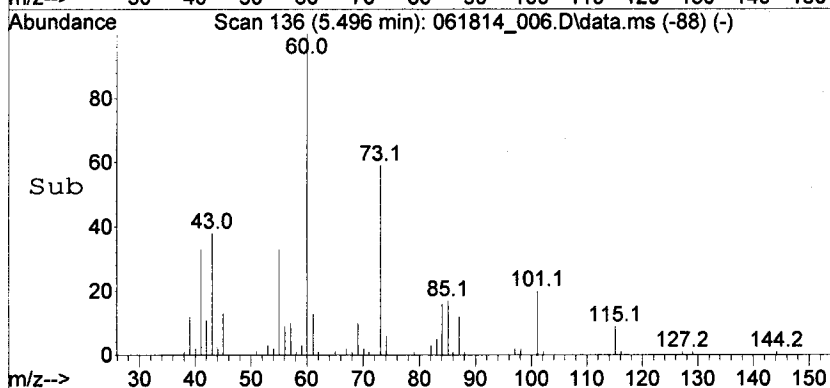
Quant Time: Jun 19 16:08:47 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids (b) (7) MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration





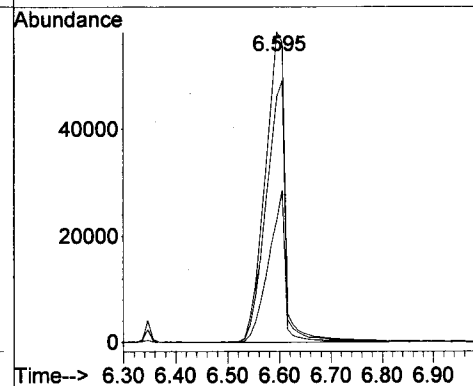
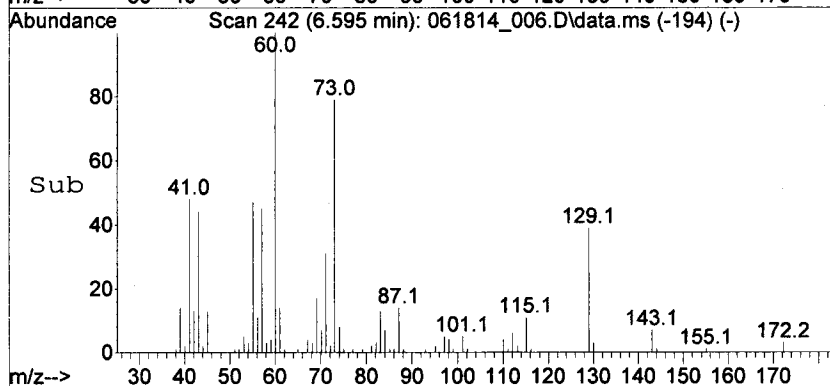
#1
 Octanoic Acid
 Concen: N.D.
 RT: 5.496 min Scan# 136
 Delta R.T. 0.001 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

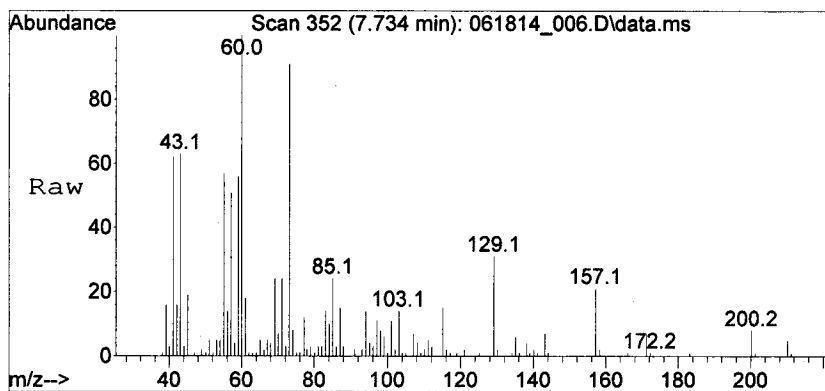
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 60 | 100 | | |
| 73 | 58.5 | 47.3 | 70.9 |
| 101 | 20.4 | 16.3 | 24.5 |



#2
 Decanoic Acid
 Concen: N.D.
 RT: 6.595 min Scan# 242
 Delta R.T. -0.003 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

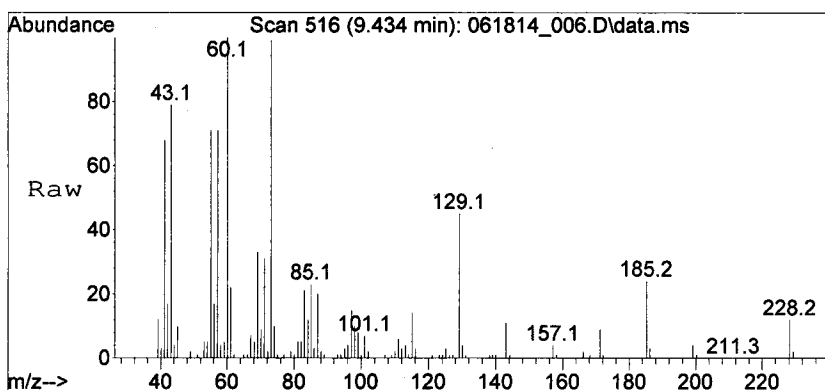
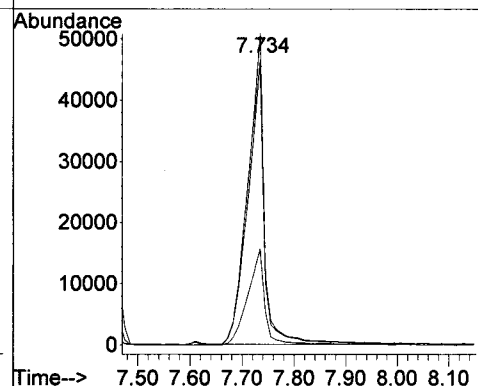
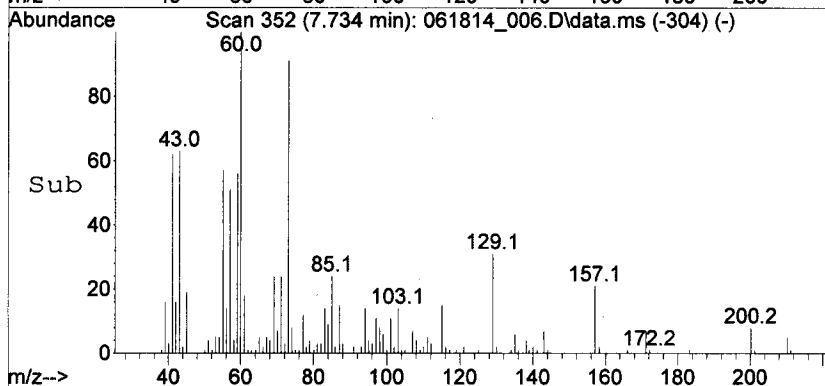
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 60 | 100 | | |
| 73 | 81.3 | 63.4 | 95.2 |
| 129 | 41.3 | 31.5 | 47.3 |





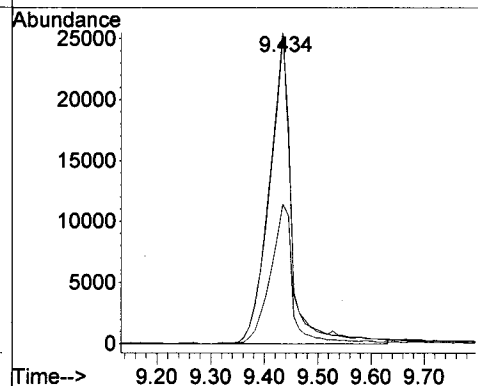
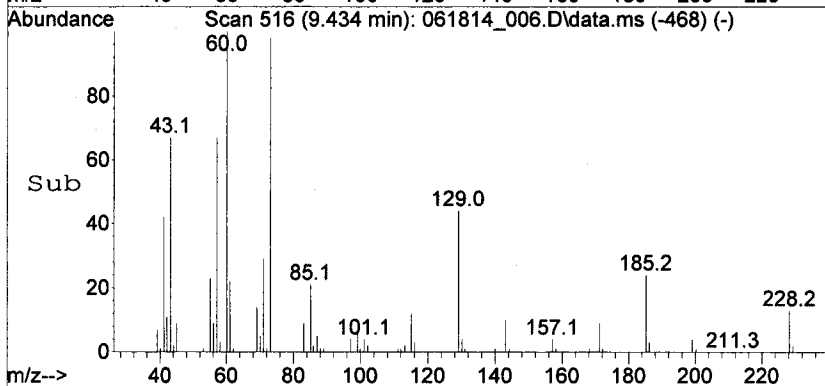
#3
Dodecanoic Acid
Concen: N.D.
RT: 7.734 min Scan# 352
Delta R.T. -0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

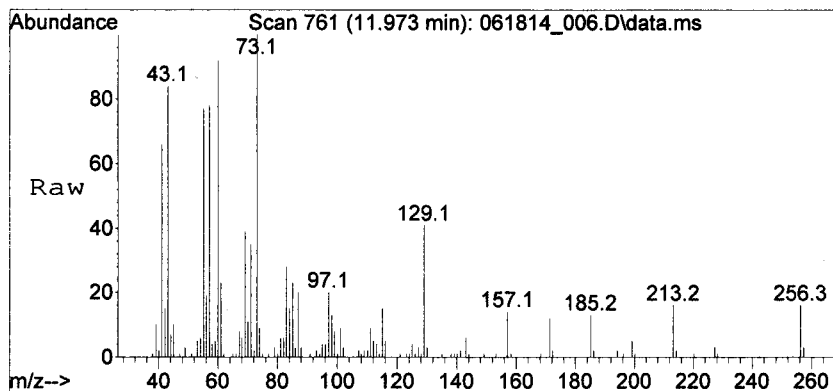
Tgt Ion: 60 Resp: 113308
Ion Ratio Lower Upper
60 / 100
73 / 90.6 73.1 109.7
129 / 31.6 24.7 37.1



#4
Tetradecanoic Acid
Concen: N.D.
RT: 9.434 min Scan# 516
Delta R.T. 0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

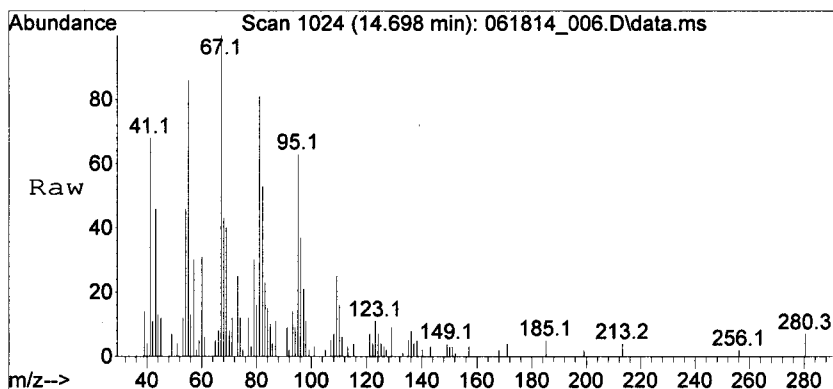
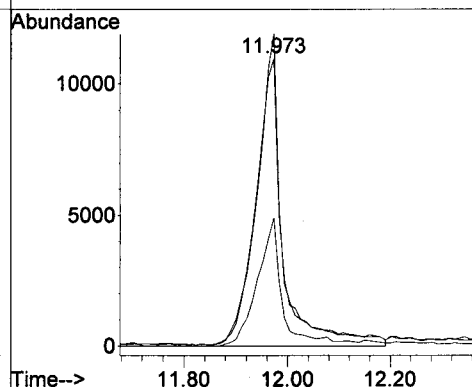
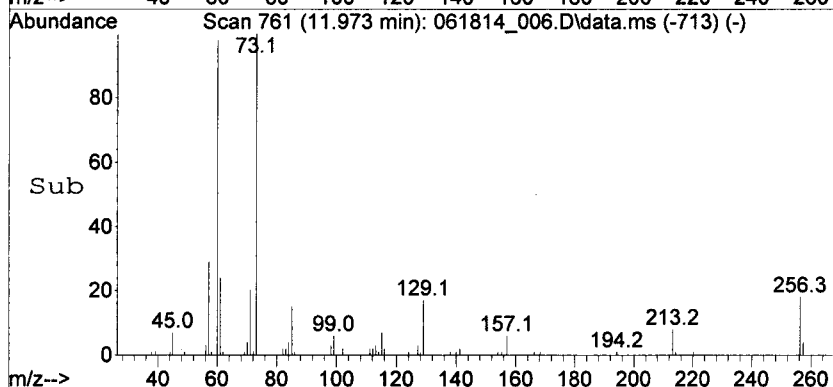
Tgt Ion: 60 Resp: 73716
Ion Ratio Lower Upper
60 / 100
73 / 100.0 79.4 119.2
129 / 44.5 35.8 53.8





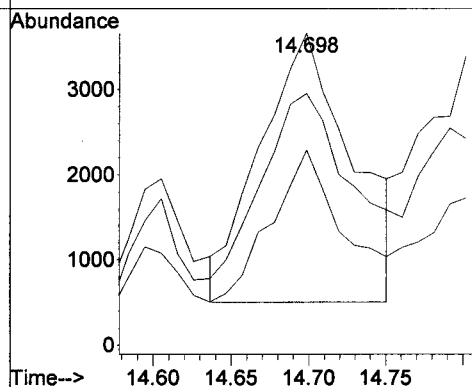
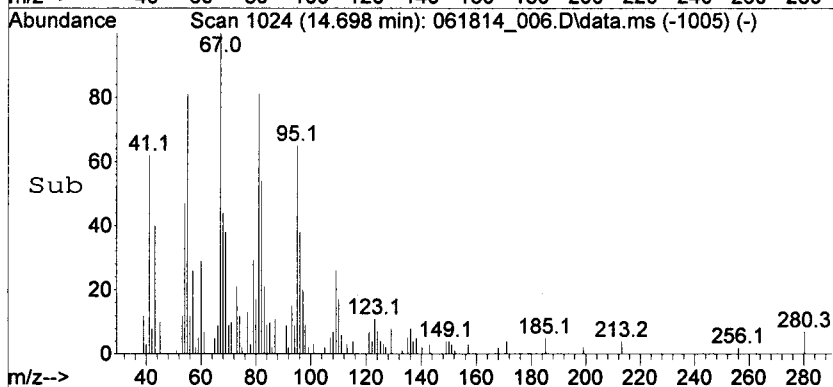
#5
Hexadecanoic Acid
Concen: N.D.
RT: 11.973 min Scan# 761
Delta R.T. 0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

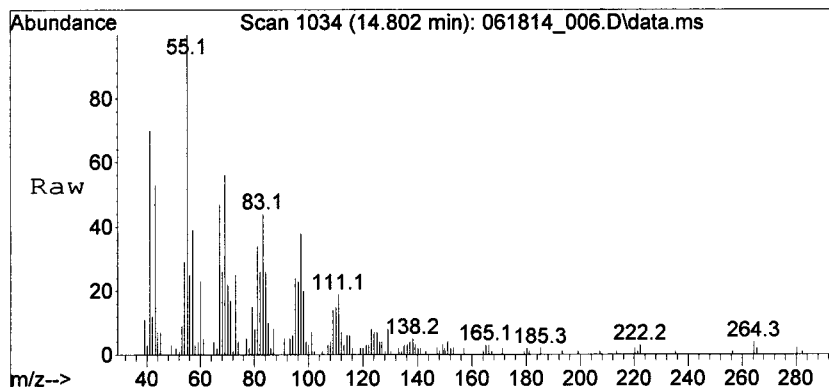
Tgt Ion: 73 Resp: 41500
Ion Ratio Lower Upper
73 / 100
60 / 97.3 73.6 110.4
129 / 38.7 32.8 49.2



#6
Linoleic Acid
Concen: N.D. m
RT: 14.698 min Scan# 1024
Delta R.T. -0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

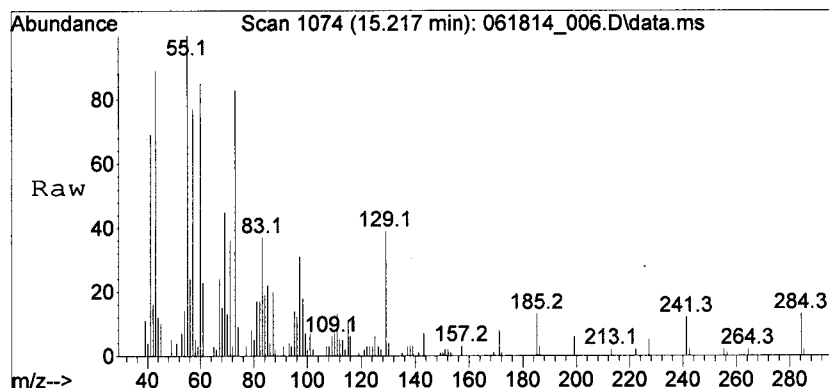
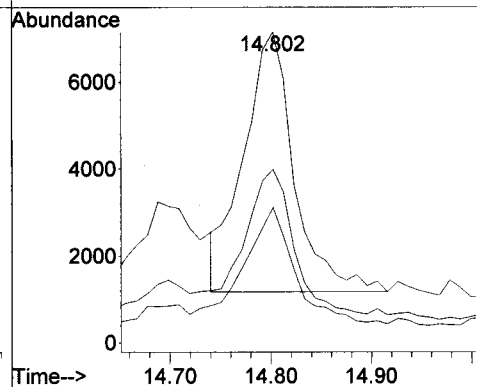
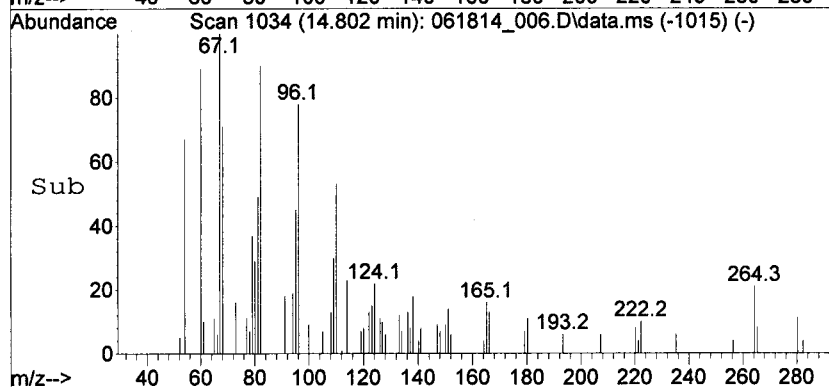
Tgt Ion: 67 Resp: 12951
Ion Ratio Lower Upper
67 / 100
81 / 87.3 64.6 97.0
95 / 57.5 50.2 75.2





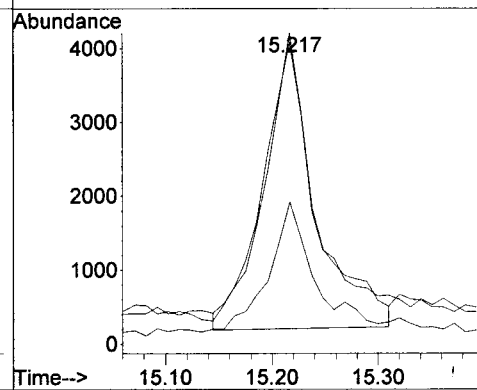
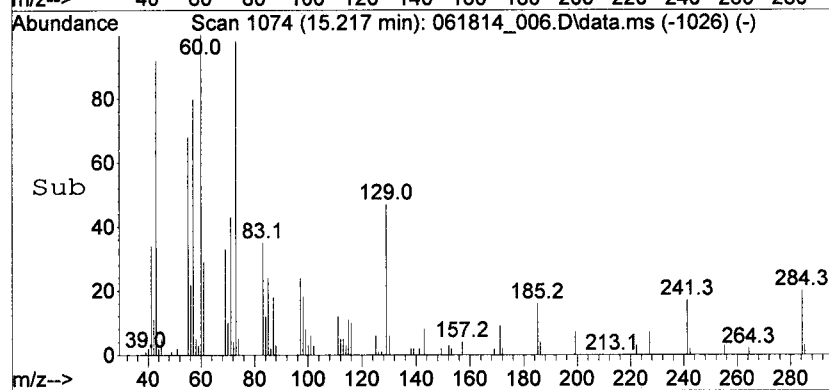
#7
Oleic Acid
Concen: N.D.
RT: 14.802 min Scan# 1034
Delta R.T. -0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

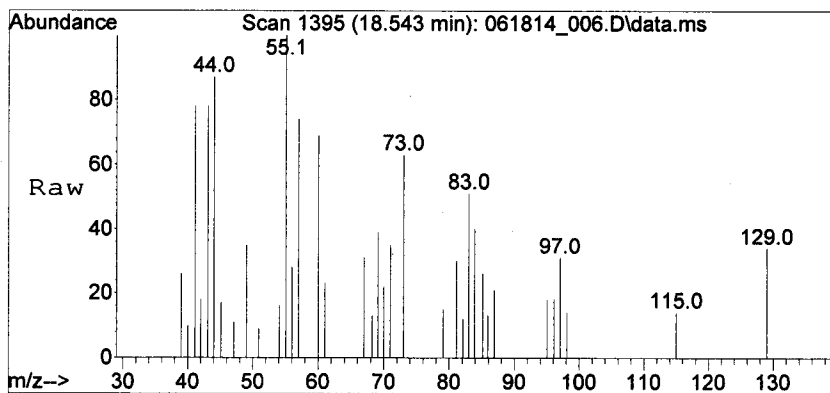
| Tgt Ion | 55 | 69 | 83 | Ratio | Lower | Upper | Resp |
|---------|------|----|----|-------|-------|-------|-------|
| 55 | 100 | | | | | | 20948 |
| 69 | 54.6 | ✓ | | 44.6 | | 67.0 | |
| 83 | 44.6 | ✓ | | 35.0 | | 52.4 | |



#8
Octadecanoic Acid
Concen: N.D. m
RT: 15.217 min Scan# 1074
Delta R.T. -0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

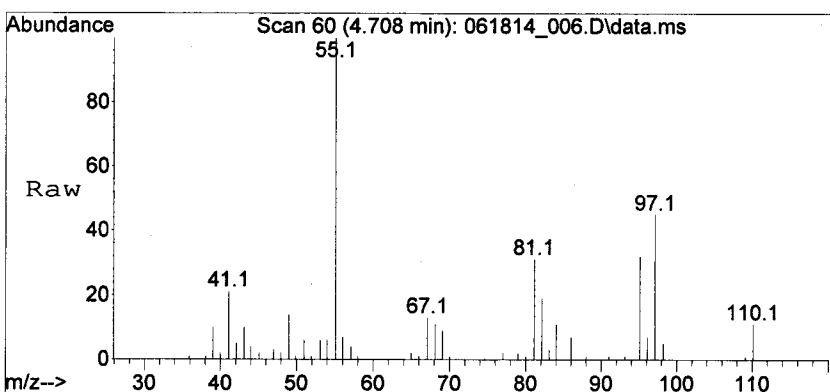
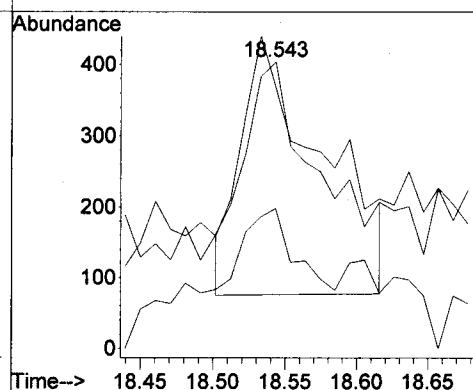
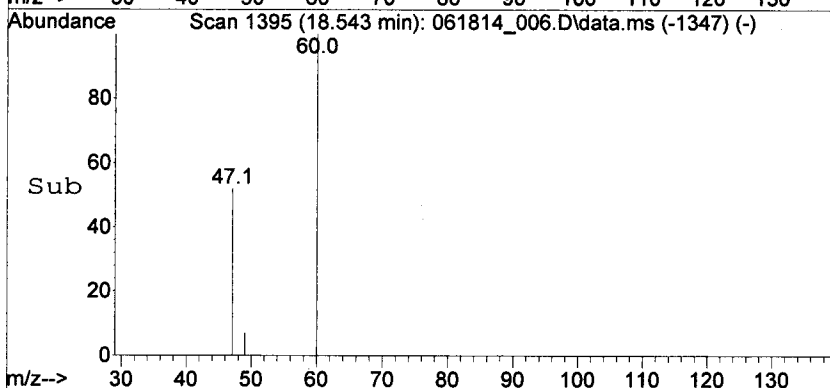
| Tgt Ion | 60 | 73 | 129 | Ratio | Lower | Upper | Resp |
|---------|------|----|-----|-------|-------|-------|-------|
| 60 | 100 | | | | | | 13382 |
| 73 | 96.1 | ✓ | | 77.8 | | 116.6 | |
| 129 | 39.8 | ✓ | | 36.6 | | 54.8 | |





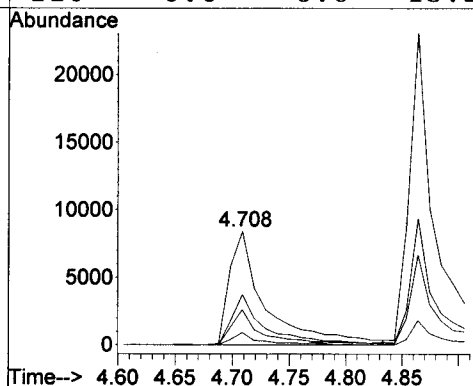
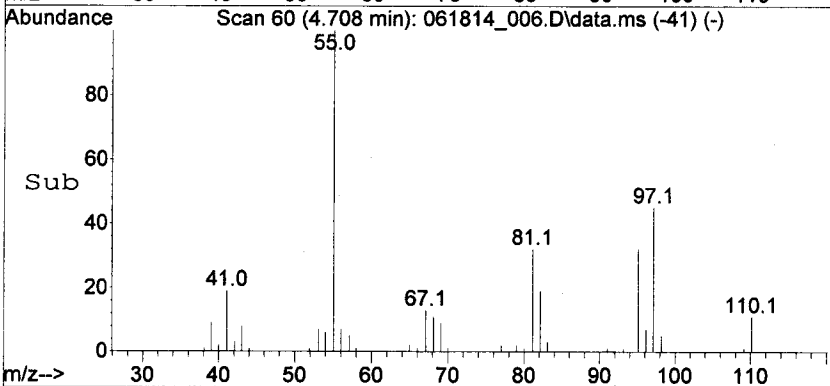
#9
 Eicosanoic Acid
 Concen: N.D. m
 RT: 18.543 min Scan# 1395
 Delta R.T. 0.001 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

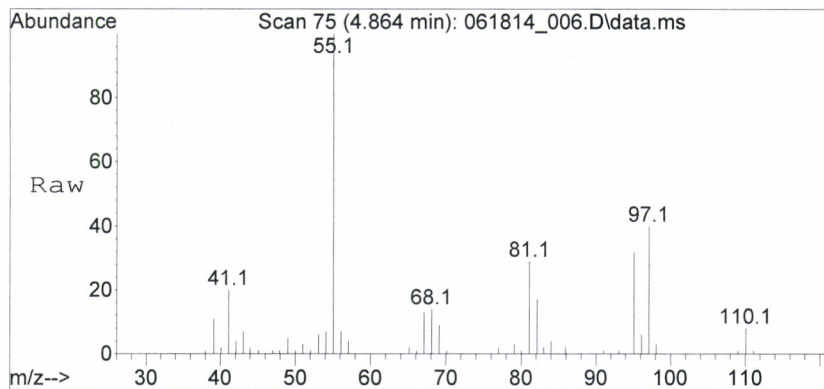
| Tgt Ion | 60 | Resp | 1280 |
|-----------|-------|-------|--------|
| Ion Ratio | Lower | Upper | |
| 60 | 100 | | |
| 73 | 70.9 | 72.9 | 109.3# |
| 129 | 73.4 | 39.2 | 58.8# |



#10
 MCHM (I)
 Concen: N.D.
 RT: 4.708 min Scan# 60
 Delta R.T. 0.000 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

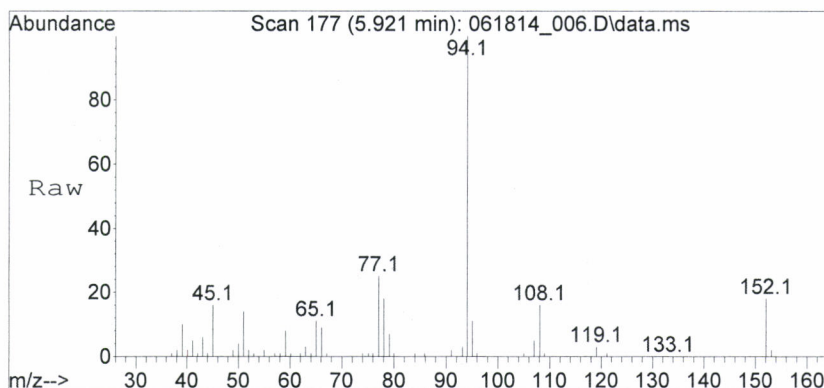
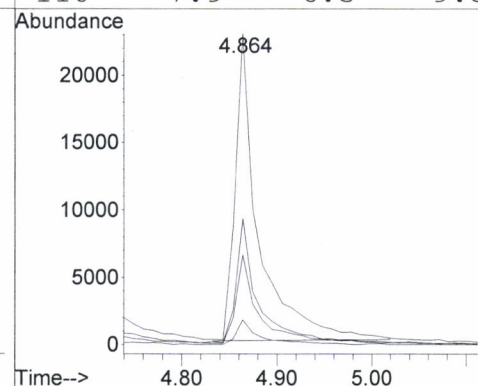
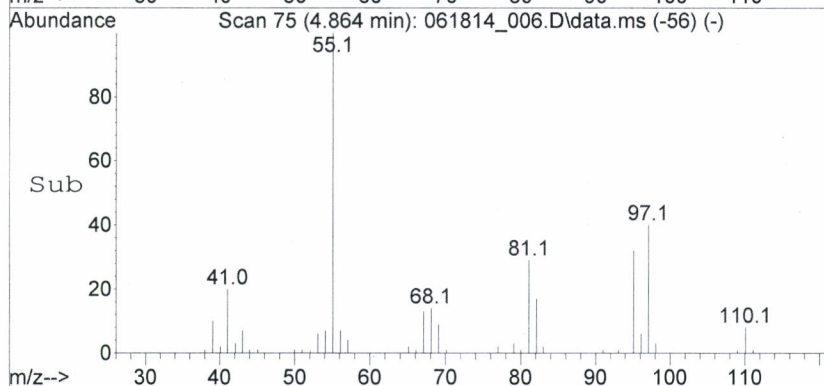
| Tgt Ion | 55 | Resp | 18815 |
|-----------|-------|-------|-------|
| Ion Ratio | Lower | Upper | |
| 55 | 100 | | |
| 97 | 41.3 | 35.7 | 53.5 |
| 81 | 27.9 | 25.0 | 37.6 |
| 110 | 8.8 | 8.8 | 13.2 |





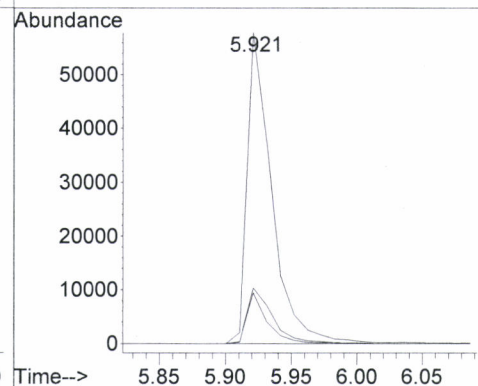
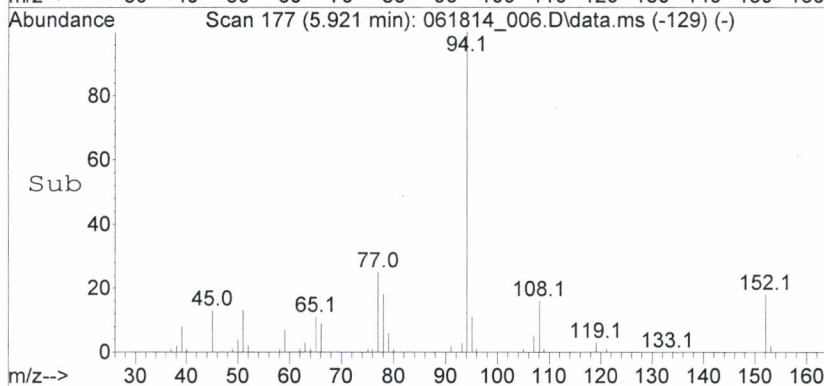
#11
MCHM (II)
Concen: N.D.
RT: 4.864 min Scan# 75
Delta R.T. -0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

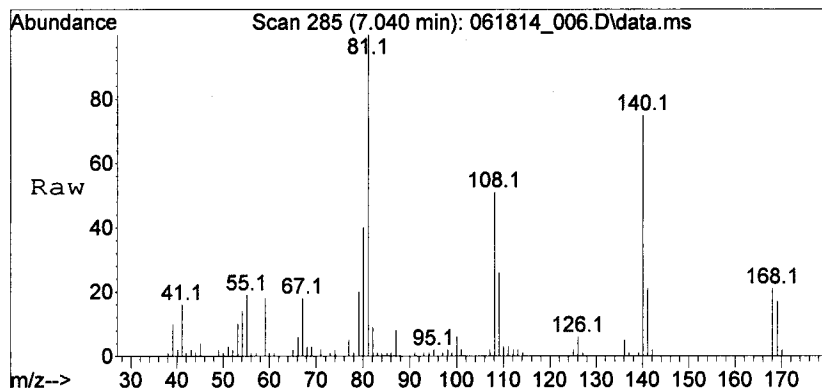
| Tgt Ion | 55 | 97 | 81 | 110 |
|-----------|-------|------|------|-----|
| Ion Ratio | 100 | 38.4 | 28.7 | 7.9 |
| Resp | 39341 | 32.4 | 23.0 | 6.3 |
| Lower | | | | |
| Upper | | 48.6 | 34.6 | 9.5 |



#12
PPH
Concen: N.D.
RT: 5.921 min Scan# 177
Delta R.T. -0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

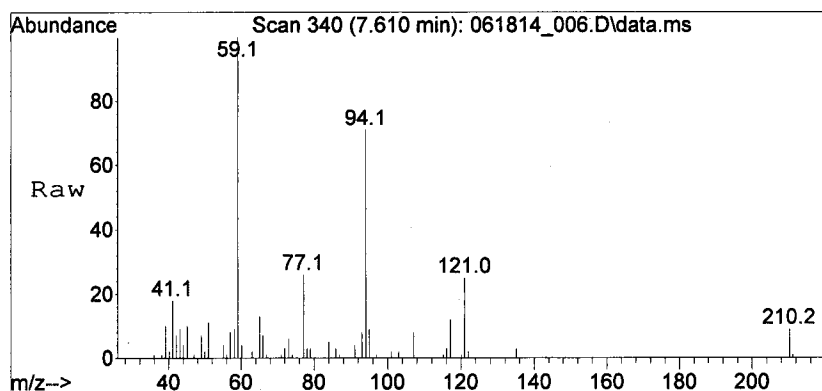
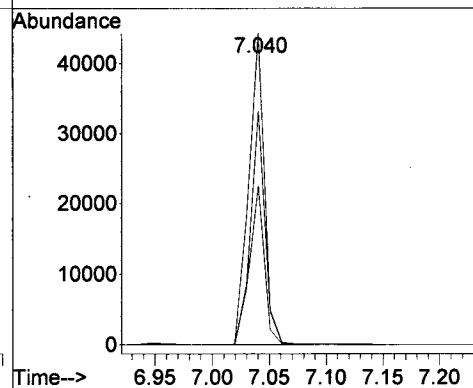
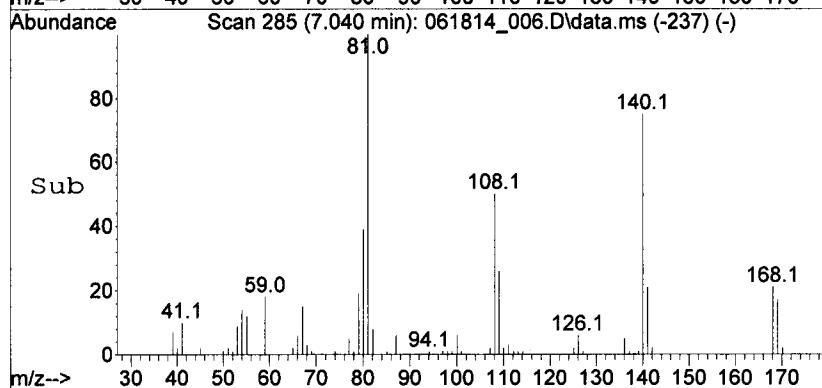
| Tgt Ion | 94 | 152 | 108 |
|-----------|-------|------|------|
| Ion Ratio | 100 | 18.5 | 13.6 |
| Resp | 75438 | 14.2 | 13.0 |
| Lower | | | |
| Upper | | 21.4 | 19.6 |





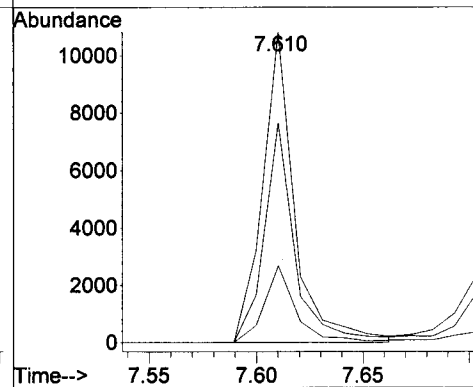
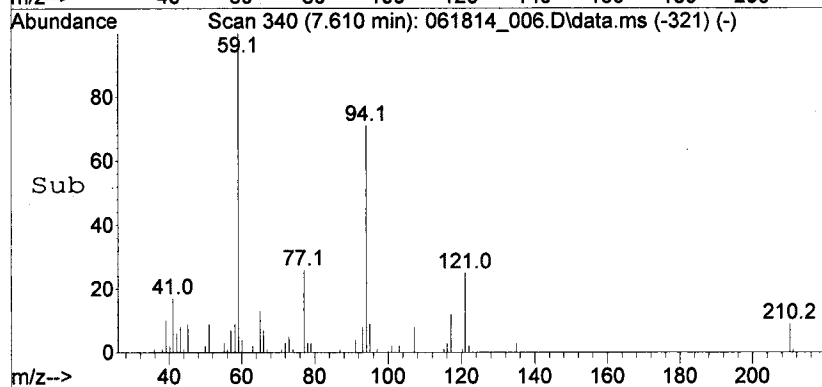
#15
DMCH-1,4-DC
Concen: N.D.
RT: 7.040 min Scan# 285
Delta R.T. 0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

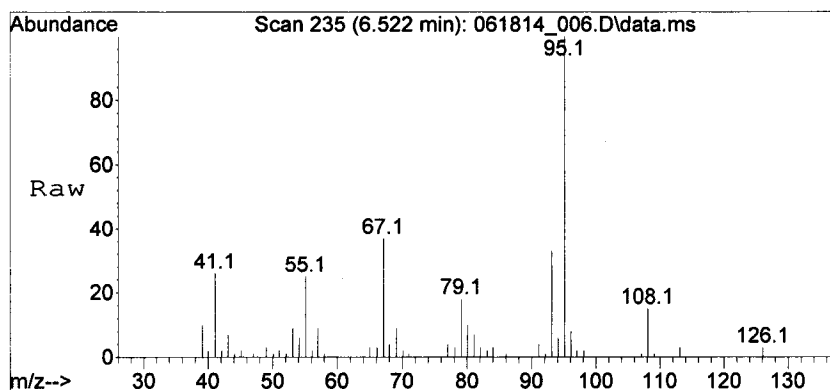
| Tgt Ion | Ratio | Resp | Lower | Upper |
|---------|-------|-------|-------|-------|
| 81 | 100 | 42484 | | |
| 108 | 48.1 | 40.6 | 61.0 | |
| 140 | 68.3 | 60.0 | 90.0 | |



#16
Di-PPH (I)
Concen: N.D.
RT: 7.610 min Scan# 340
Delta R.T. 0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

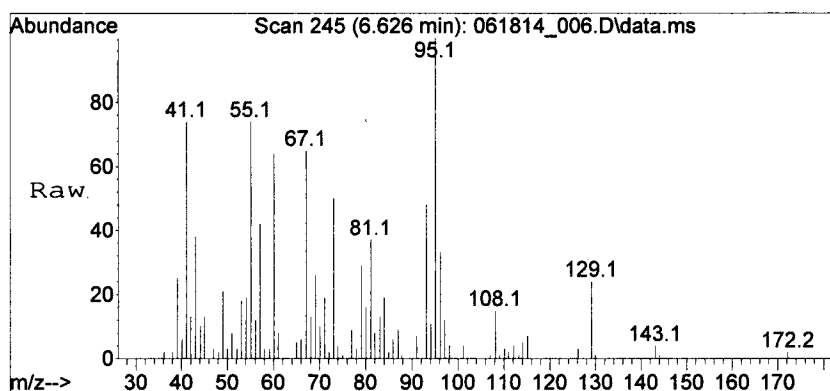
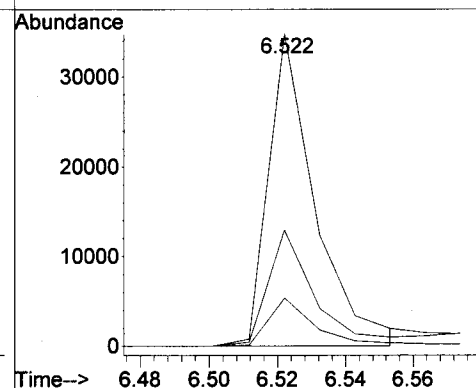
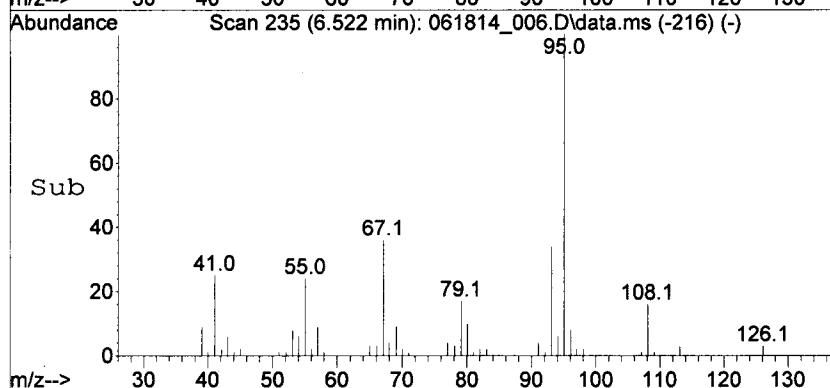
| Tgt Ion | Ratio | Resp | Lower | Upper |
|---------|-------|-------|-------|-------|
| 59 | 100 | 11307 | | |
| 94 | 67.6 | 56.6 | 85.0 | |
| 121 | 24.7 | 19.9 | 29.9 | |





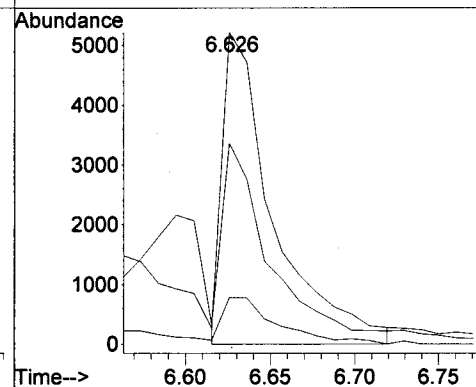
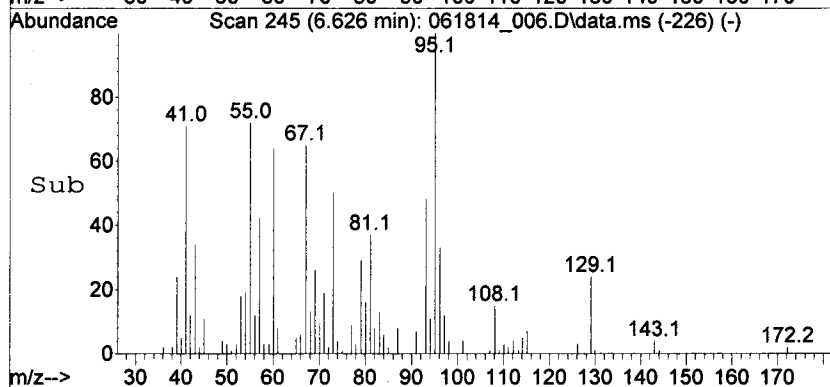
#13
1,4-CHDM (I)
Concen: N.D. m
RT: 6.522 min Scan# 235
Delta R.T. 0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

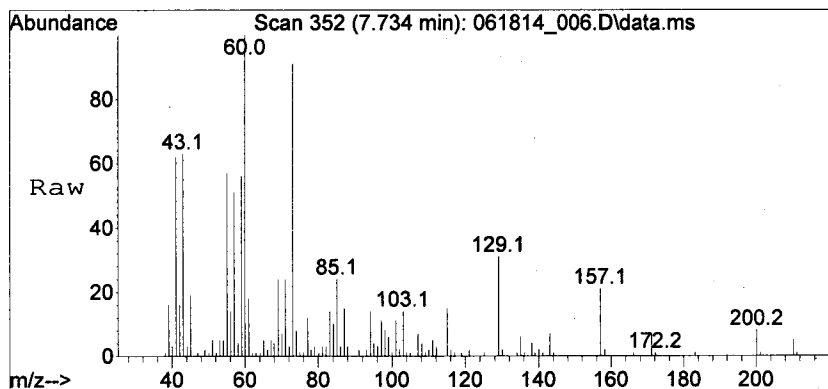
Tgt Ion: 95 Resp: 33100
Ion / Ratio Lower Upper
95 / 100
67 / 37.3 29.7 44.5
108 / 16.9 12.4 18.6



#14
1,4-CHDM (II)
Concen: N.D. m
RT: 6.626 min Scan# 245
Delta R.T. -0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

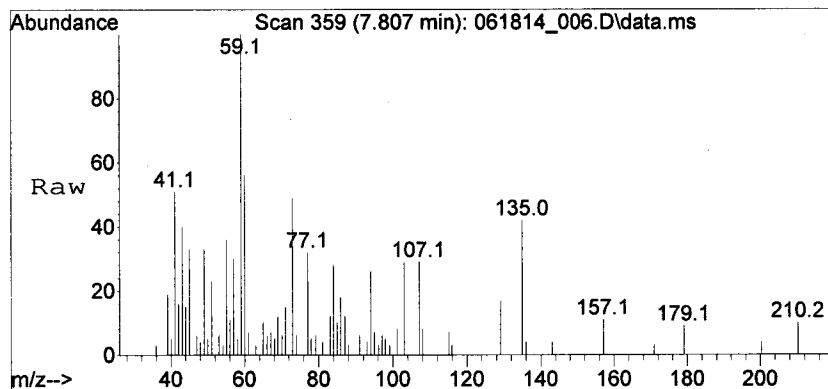
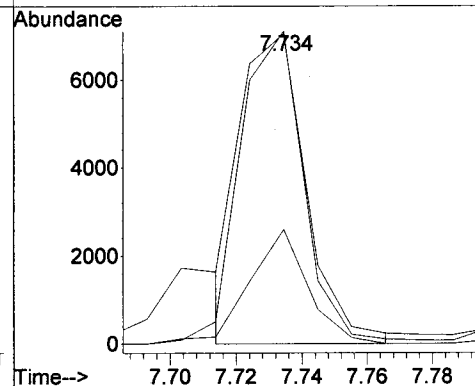
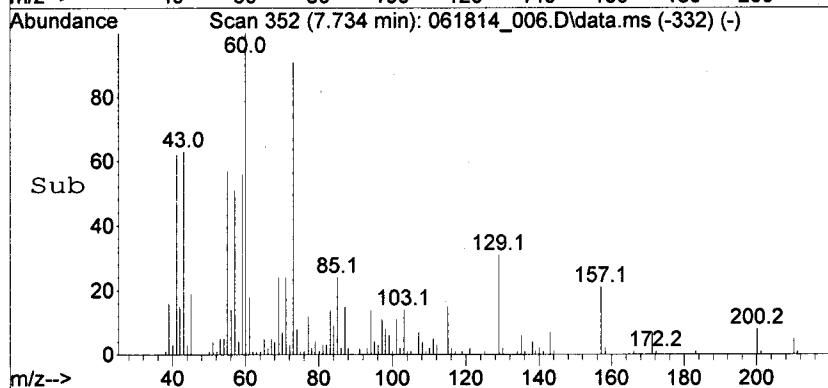
Tgt Ion: 95 Resp: 10962
Ion / Ratio Lower Upper
95 / 100
67 / 61.5 51.6 77.4
108 / 16.9 12.0 18.0





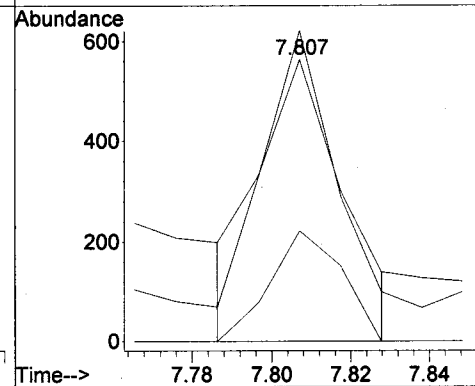
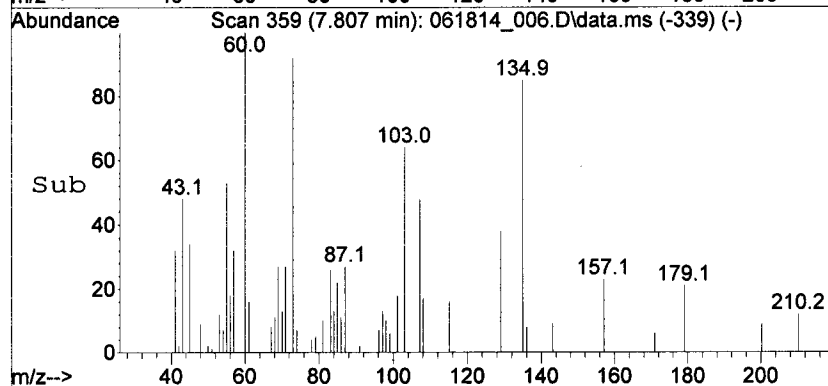
#17
di-PPH (II)
Concen: N.D. m
RT: 7.734 min Scan# 352
Delta R.T. 0.003 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

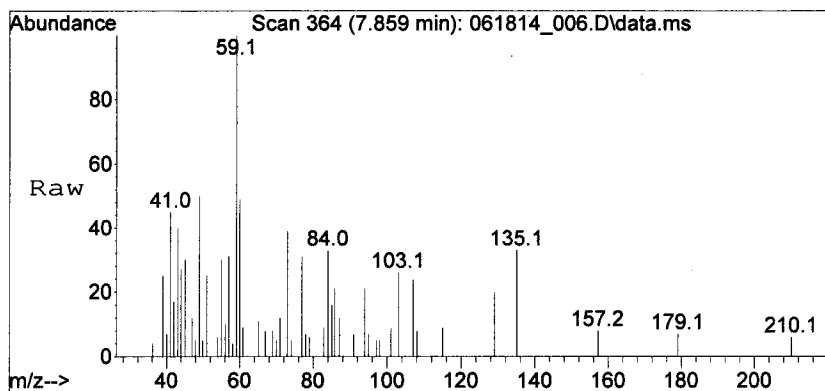
| Tgt Ion | 94 | 103 | 210 | Ratio | Lower | Upper | Resp |
|---------|------|-----|-----|-------|-------|-------|------|
| 94 | 100 | | | | | | 9848 |
| 103 | 98.6 | | | | 81.0 | 121.4 | |
| 210 | 33.1 | | | | 31.5 | 47.3 | |



#18
di-PPH (III)
Concen: N.D. m
RT: 7.807 min Scan# 359
Delta R.T. 0.003 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

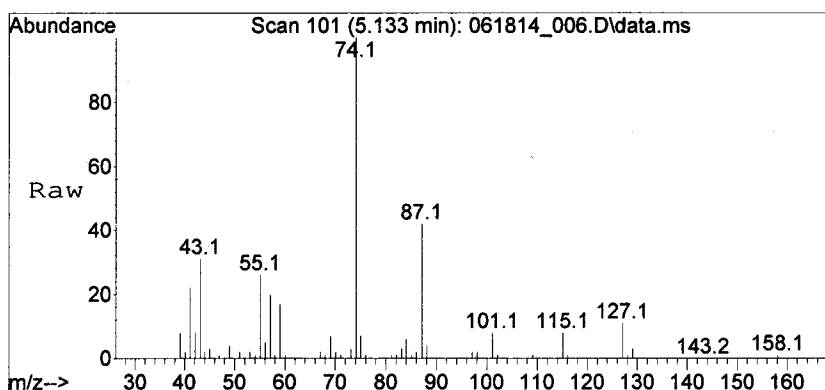
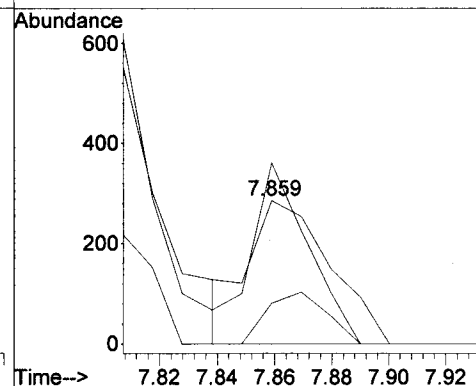
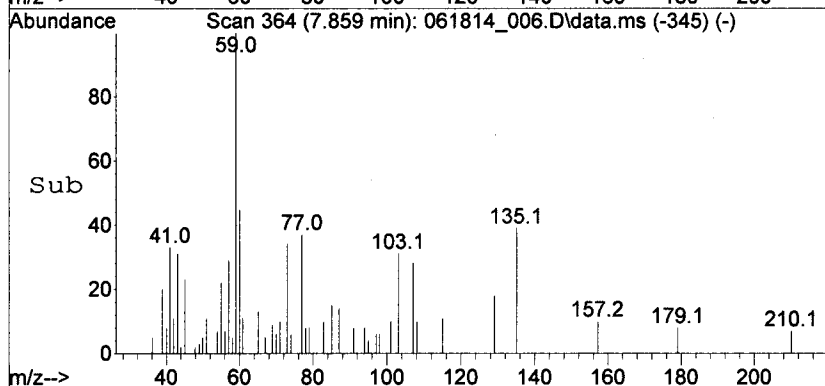
| Tgt Ion | 94 | 103 | 210 | Ratio | Lower | Upper | Resp |
|---------|-------|-----|-----|-------|-------|-------|------|
| 94 | 100 | | | | | | 831 |
| 103 | 105.5 | | | | 88.2 | 132.4 | |
| 210 | 33.9 | | | | 31.5 | 47.3 | |





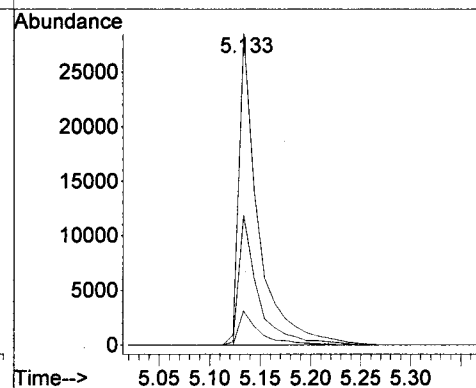
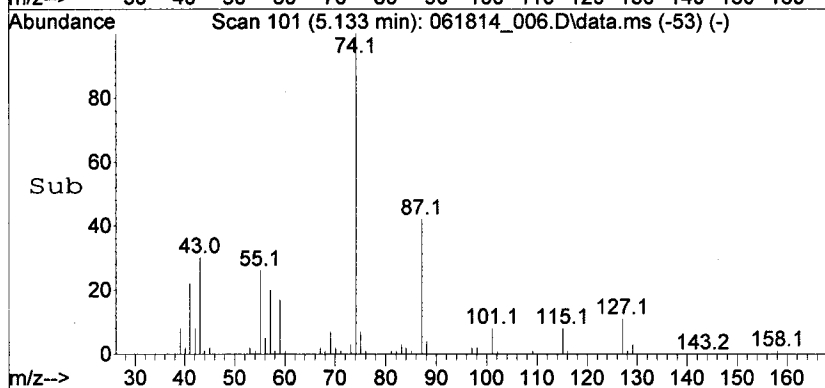
#19
di-PPH (IV)
Concen: N.D. m
RT: 7.859 min Scan# 364
Delta R.T. -0.003 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

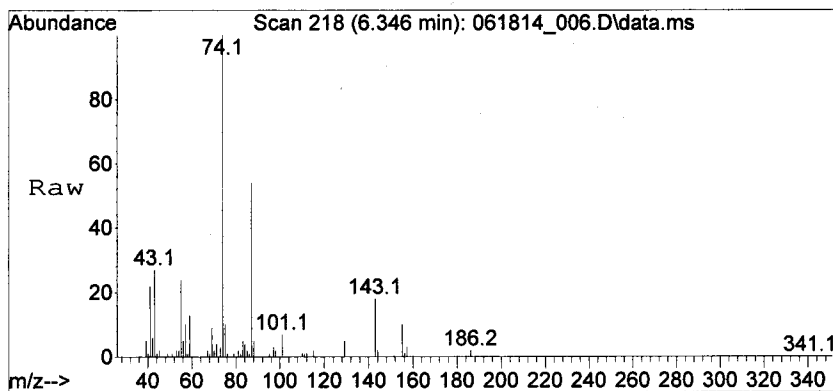
Tgt Ion: 94 Resp: 562
Ion Ratio Lower Upper
94 100 /
103 87.2 / 101.0 151.4#
210 26.5 / 22.6 34.0



#20
Octanoic Acid-ME
Concen: N.D.
RT: 5.133 min Scan# 101
Delta R.T. -0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

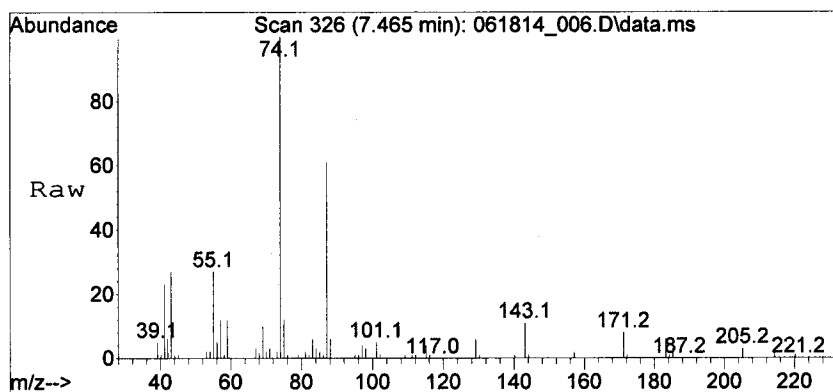
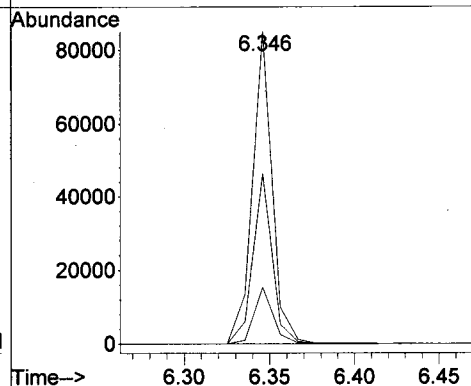
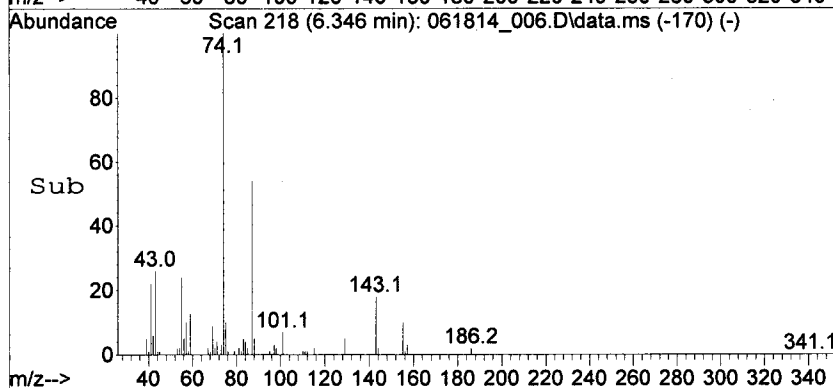
Tgt Ion: 74 Resp: 37962
Ion Ratio Lower Upper
74 100 \ /
87 41.8 \ 33.3 49.9
127 11.7 \ 8.7 13.1





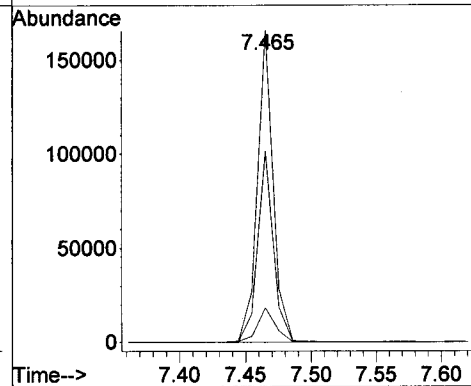
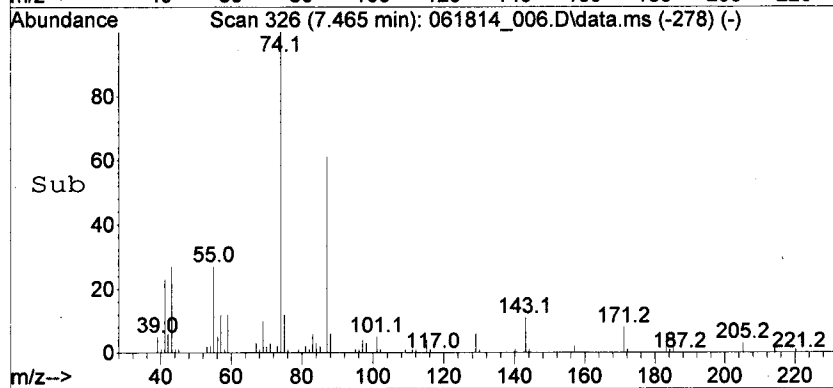
#21
Decanoic Acid-ME
Concen: N.D.
RT: 6.346 min Scan# 218
Delta R.T. 0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

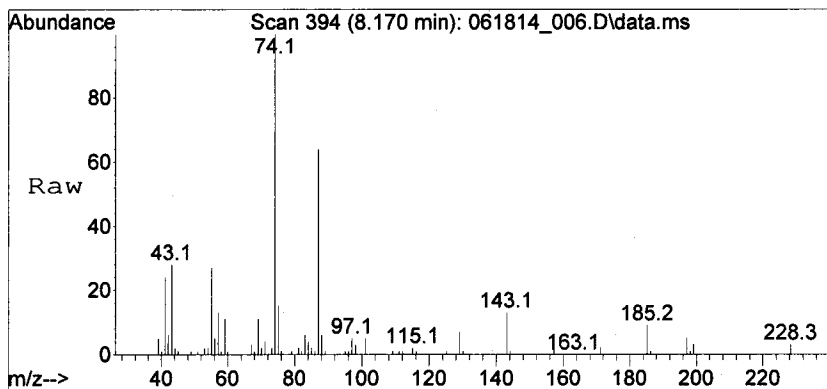
Tgt Ion: 74 Resp: 68466
Ion Ratio Lower Upper
74 100 /
87 53.4 / 43.6 65.4
143 17.4 / 14.5 21.7



#22
Dodecanoic Acid-ME
Concen: N.D.
RT: 7.465 min Scan# 326
Delta R.T. 0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

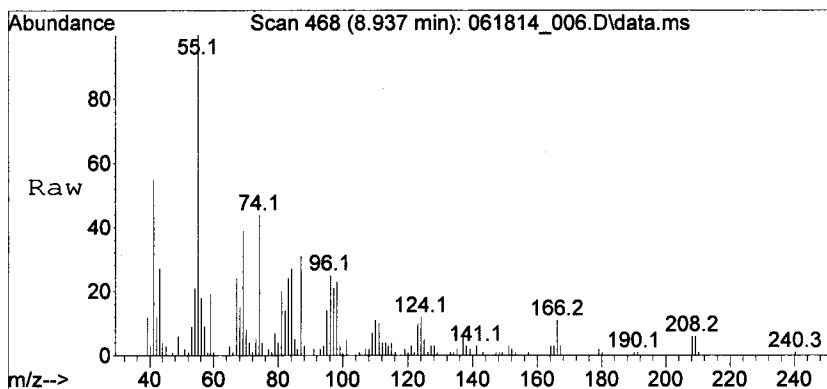
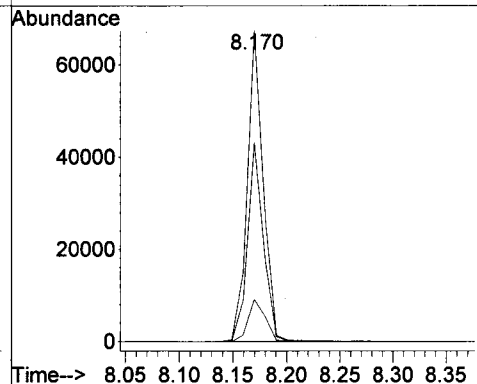
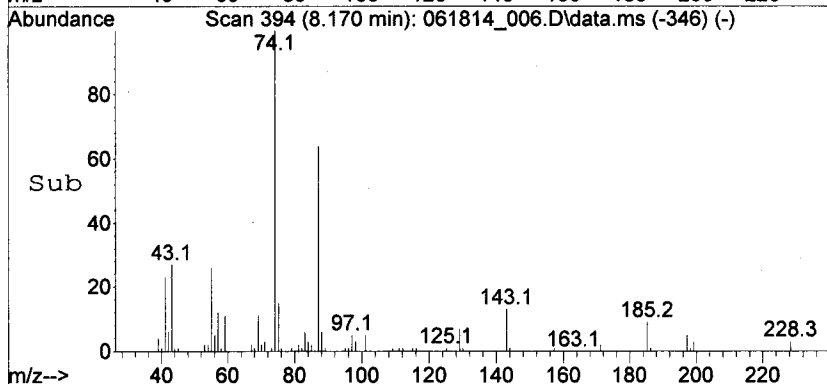
Tgt Ion: 74 Resp: 138676
Ion Ratio Lower Upper
74 /100
87 / 61.3 49.0 73.4
143 / 12.7 9.0 13.4





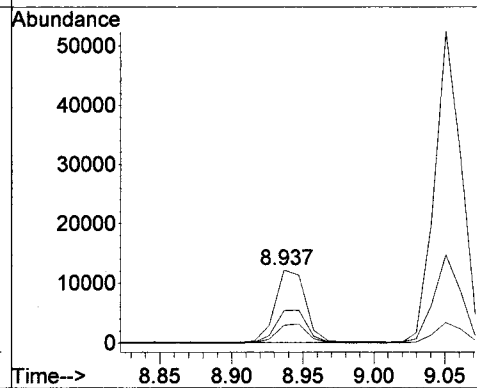
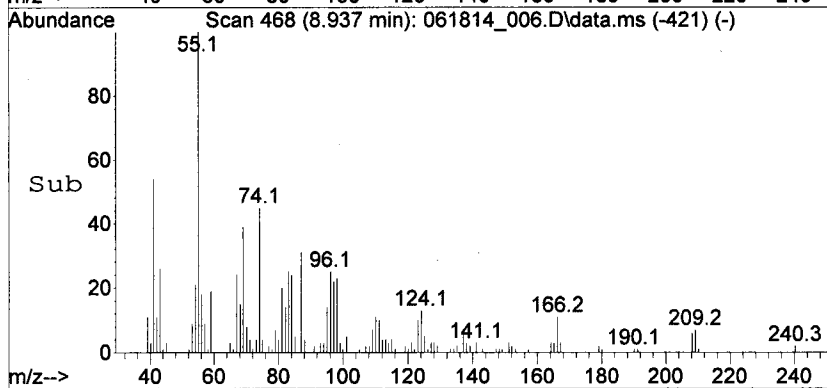
#23
 Tridecanoic Acid-ME
 Concen: N.D.
 RT: 8.170 min Scan# 394
 Delta R.T. 0.002 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

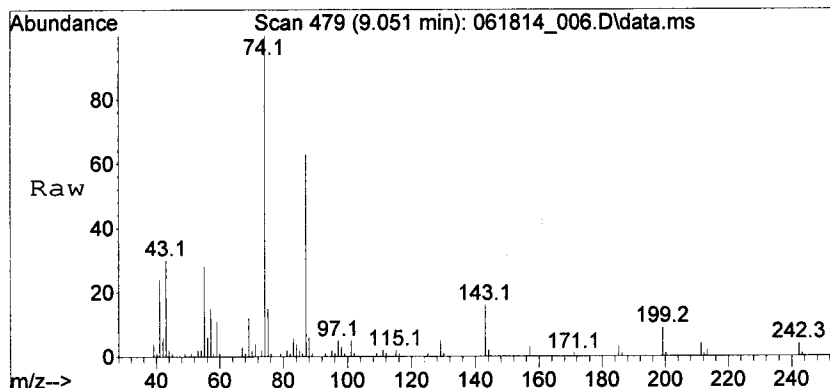
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 74 | 100 | | |
| 87 | 63.8 | 51.1 | 76.7 |
| 143 | 14.4 | 10.7 | 16.1 |



#24
 Myristolic Acid-ME
 Concen: N.D.
 RT: 8.937 min Scan# 468
 Delta R.T. -0.010 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

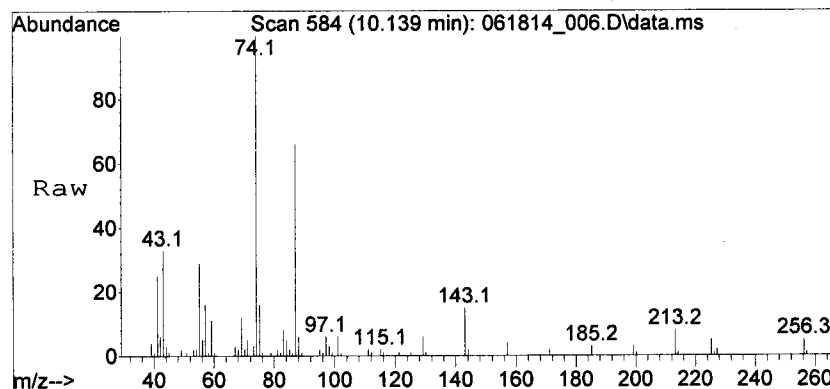
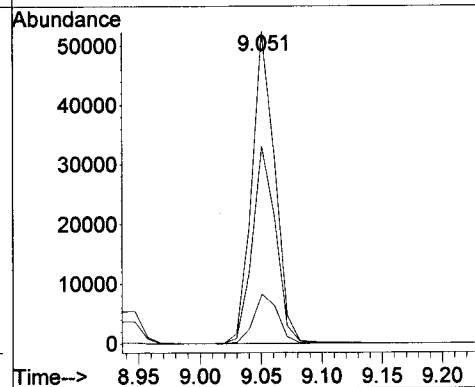
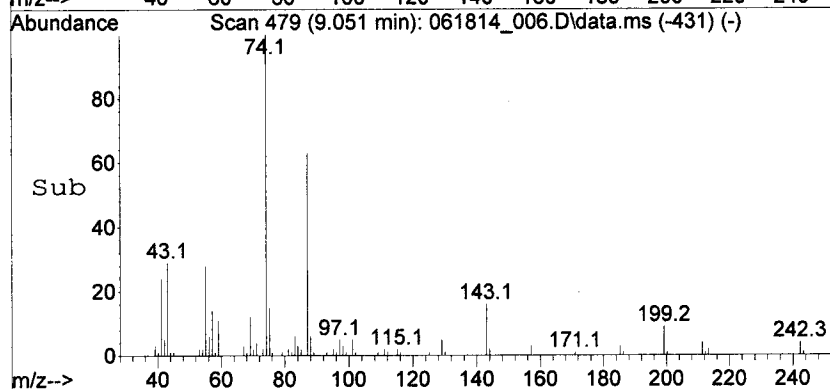
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 55 | 100 | | |
| 74 | 45.8 | 38.8 | 58.2 |
| 83 | 25.6 | 22.5 | 33.7 |





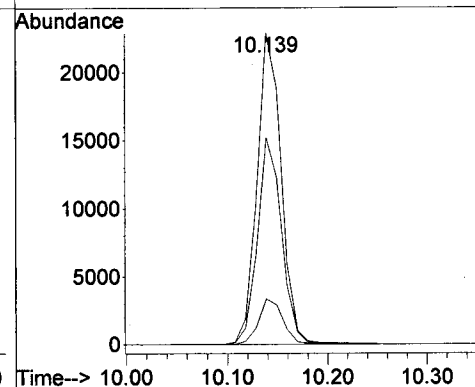
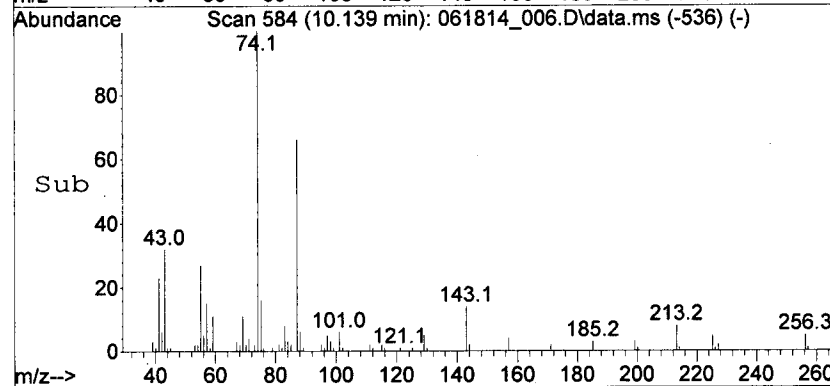
#25
Tetradecanoic Acid-ME
Concen: N.D.
RT: 9.051 min Scan# 479
Delta R.T. -0.000 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

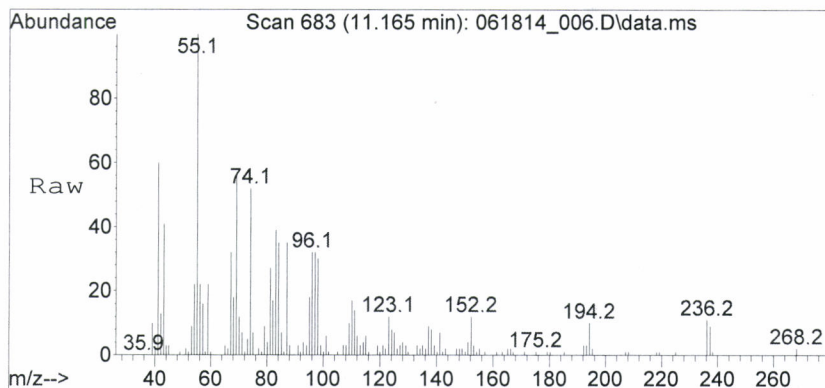
Tgt Ion: 74 Resp: 69063
Ion Ratio Lower Upper
74 100
87 64.1 50.5 75.7
143 16.6 12.6 19.0



#26
Pentadecanoic Acid-ME
Concen: N.D.
RT: 10.139 min Scan# 584
Delta R.T. -0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

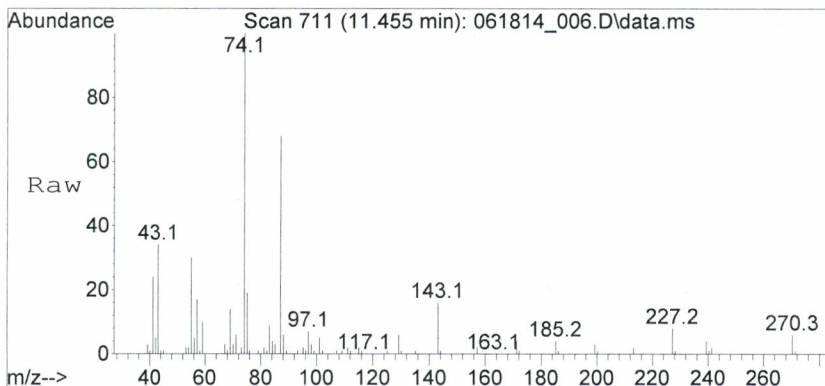
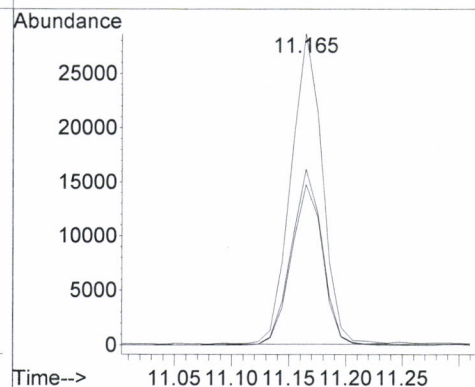
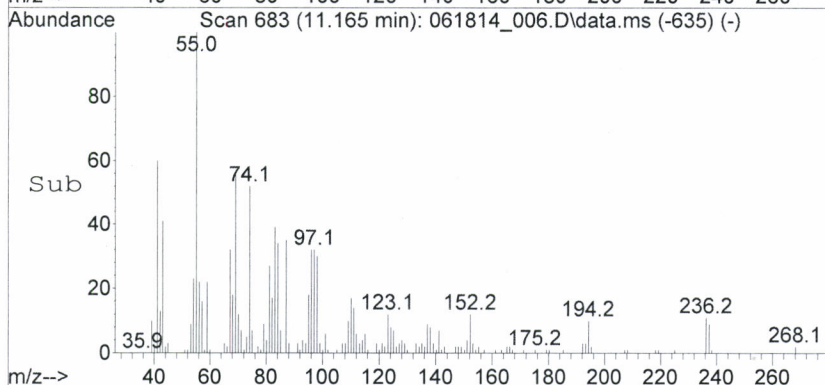
Tgt Ion: 74 Resp: 38455
Ion Ratio Lower Upper
74 100
87 66.0 53.0 79.6
143 14.7 11.8 17.6





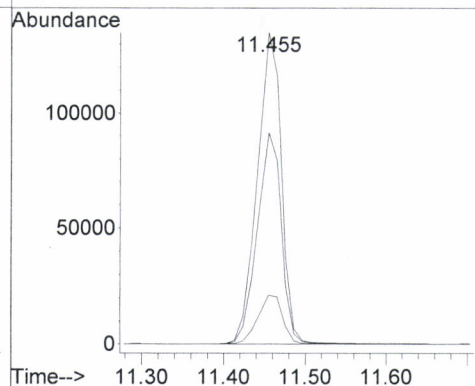
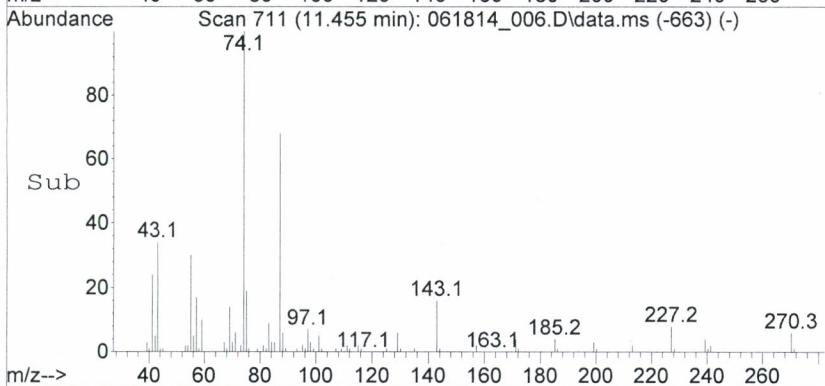
#27
 Palmitoleic Acid-ME, DH.7/25/14
 Concen: N.D.
 RT: 11.165 min Scan# 683
 Delta R.T. -0.002 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

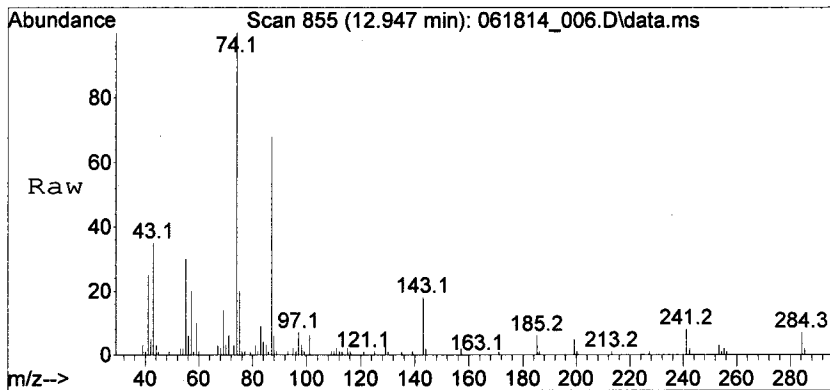
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 55 | 100 | | |
| 69 | 55.9 | 45.2 | 67.8 |
| 74 | 51.5 | 41.2 | 61.8 |



#28
 Hexadecanoic Acid-ME
 Concen: N.D.
 RT: 11.455 min Scan# 711
 Delta R.T. -0.002 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

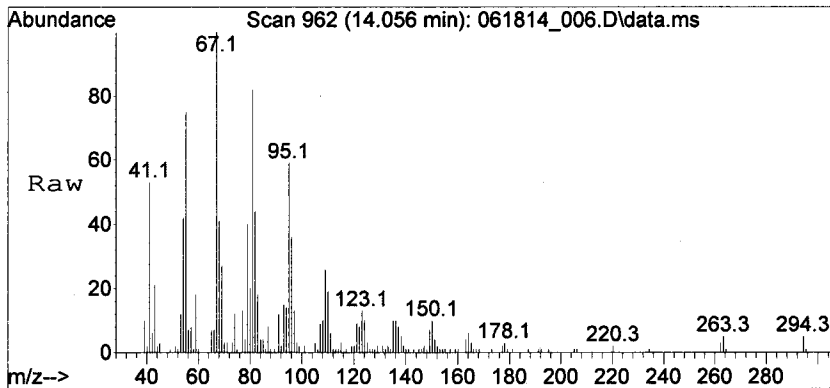
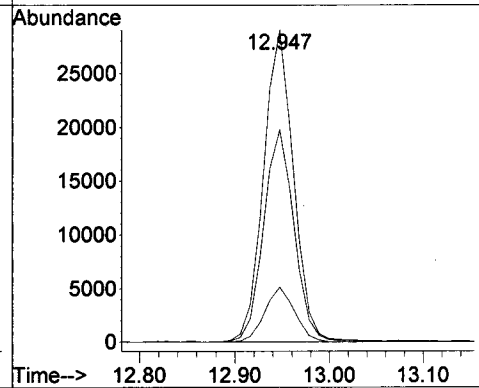
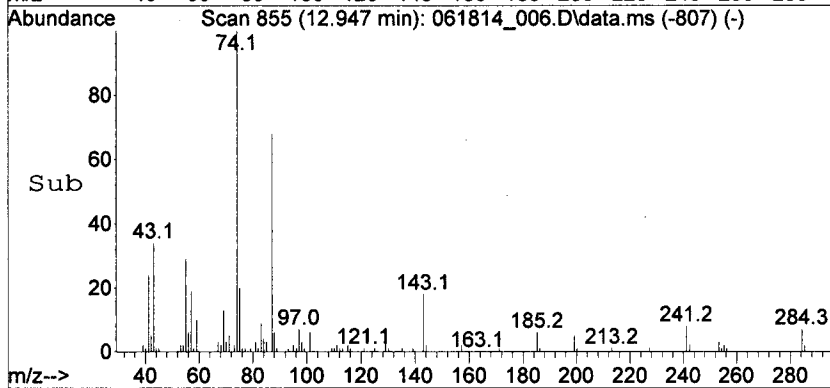
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 74 | 100 | | |
| 87 | 67.7 | 54.2 | 81.2 |
| 143 | 16.2 | 12.6 | 18.8 |





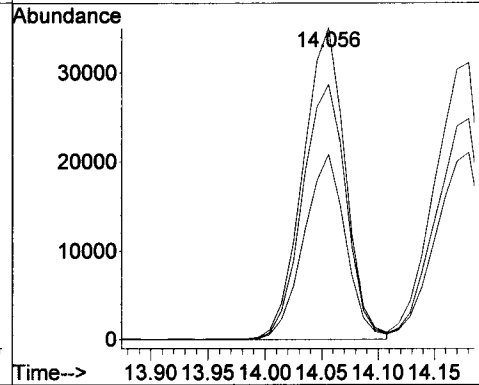
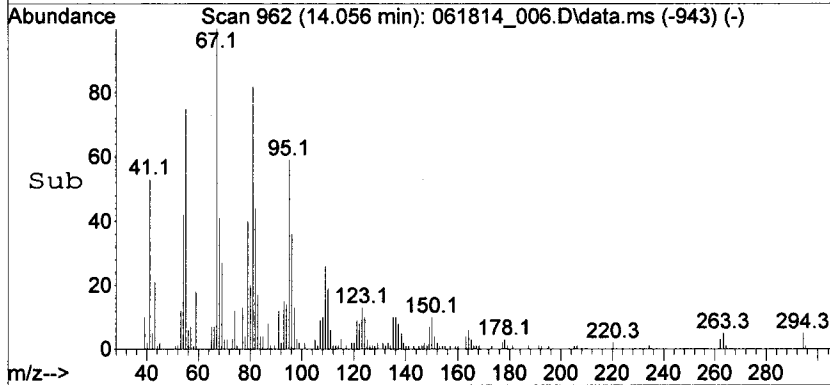
#29
 Heptadecanoic Acid-ME
 Concen: N.D.
 RT: 12.947 min Scan# 855
 Delta R.T. 0.001 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

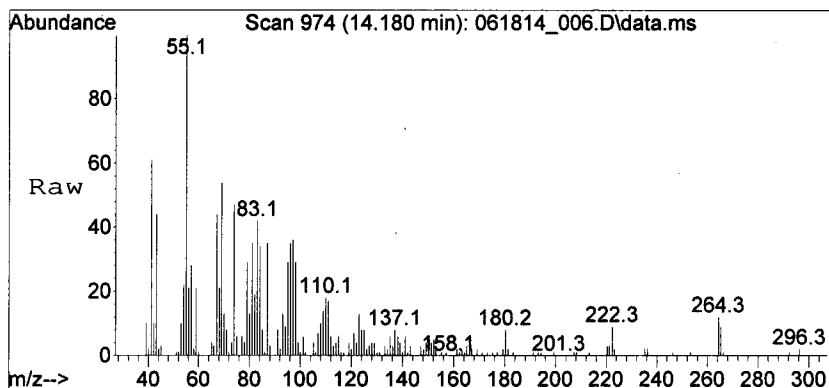
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 74 | 100 | | |
| 87 | 69.2 | 54.5 | 81.7 |
| 143 | 17.5 | 14.1 | 21.1 |



#30
 Linoleic Acid-ME
 Concen: N.D.
 RT: 14.056 min Scan# 962
 Delta R.T. -0.001 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

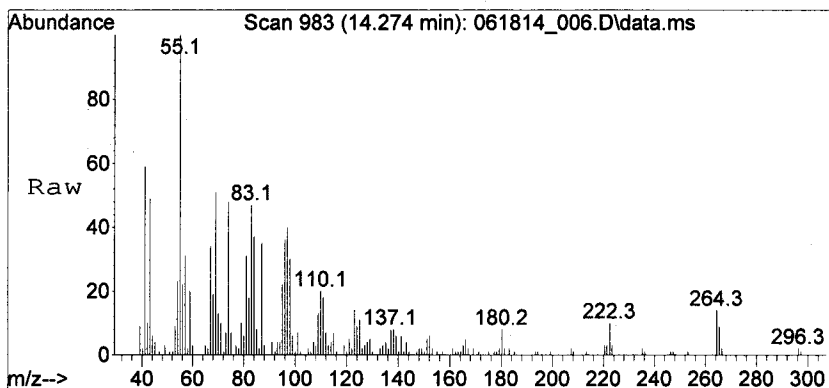
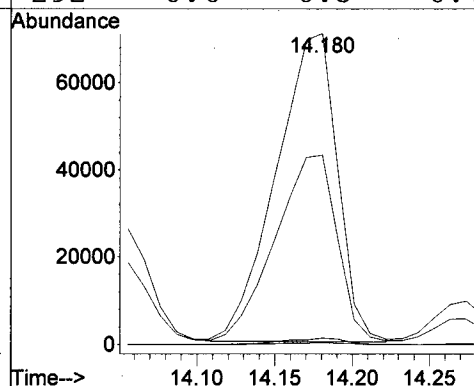
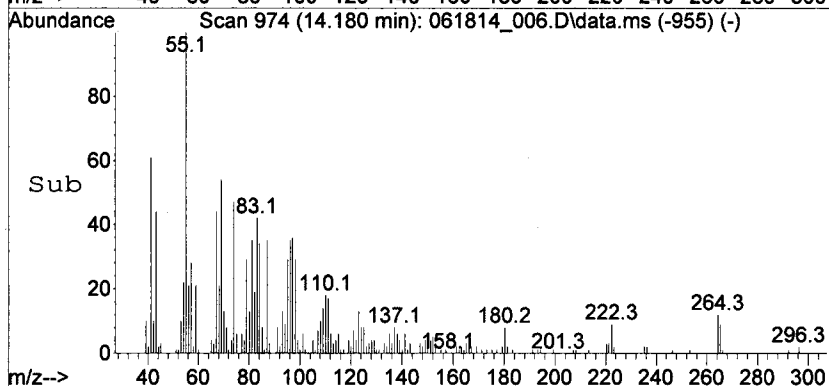
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 67 | 100 | | |
| 81 | 84.3 | 65.5 | 98.3 |
| 95 | 58.5 | 47.5 | 71.3 |





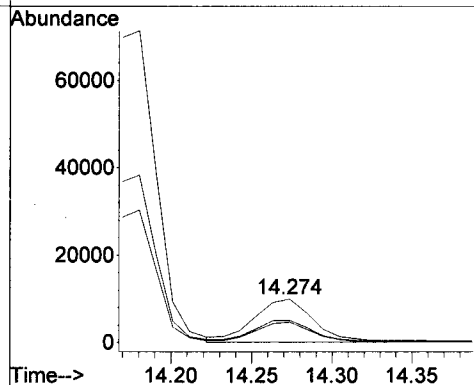
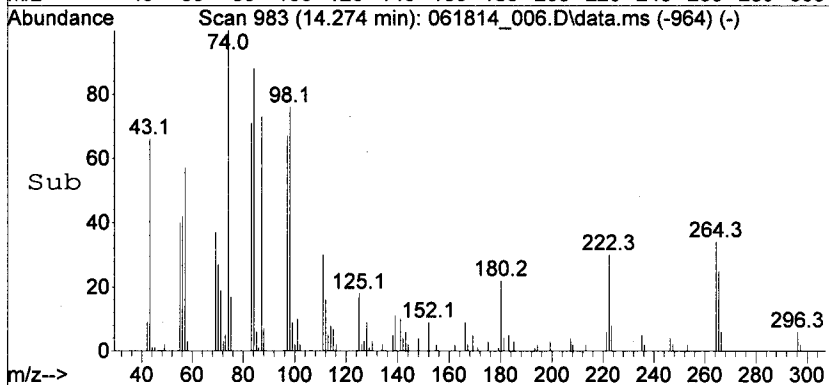
#31
 Linolenic/Oleic Acid-MEs
 Concen: N.D.
 RT: 14.180 min Scan# 974
 Delta R.T. 0.000 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

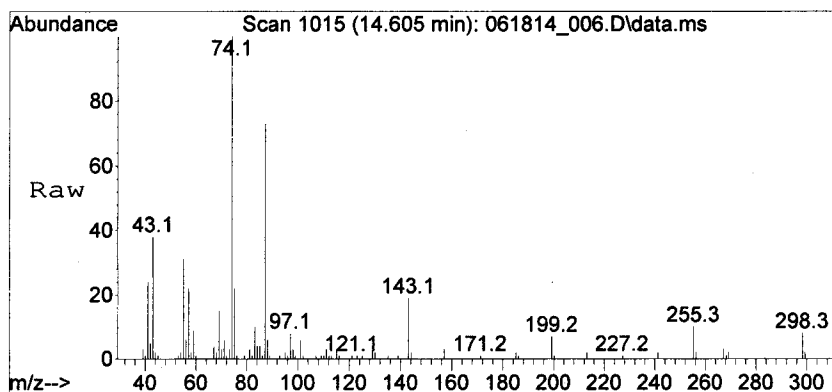
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 55 | 100 | | |
| 41 | 61.6 | 48.6 | 73.0 |
| 296 | 1.9 | 1.7 | 2.5 |
| 292 | 0.6 | 0.5 | 0.7 |



#32
 Elaidic Acid-ME
 Concen: N.D. m
 RT: 14.274 min Scan# 983
 Delta R.T. 0.001 min
 Lab File: 061814_006.D
 Acq: 18 Jun 2014 11:24 pm

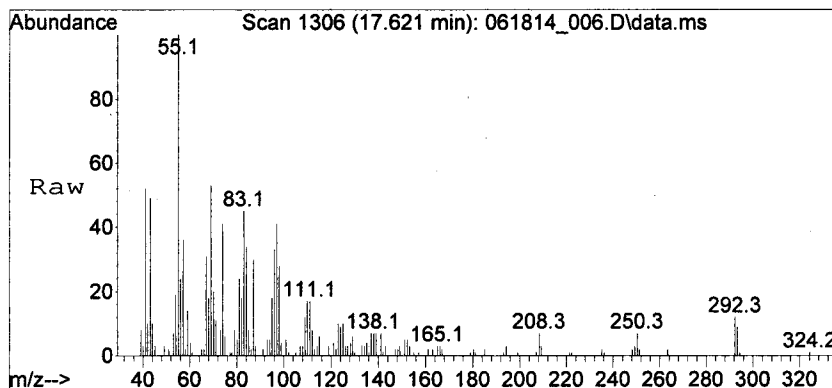
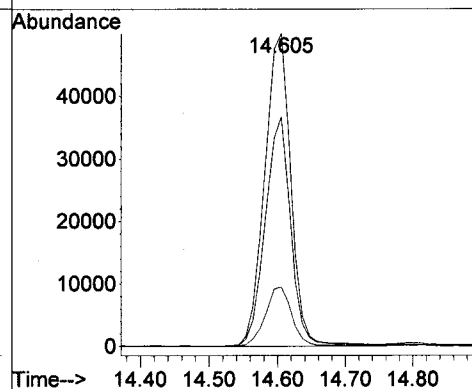
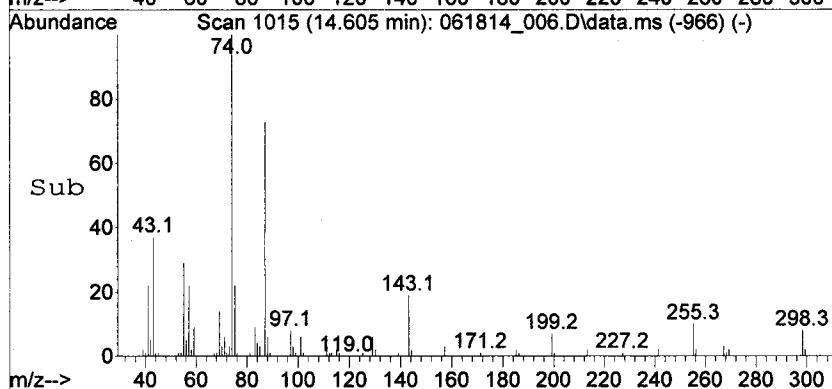
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 55 | 100 | | |
| 69 | 50.3 | 40.9 | 61.3 |
| 83 | 43.3 | 37.7 | 56.5 |





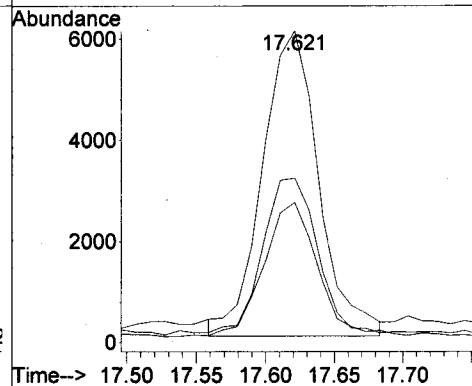
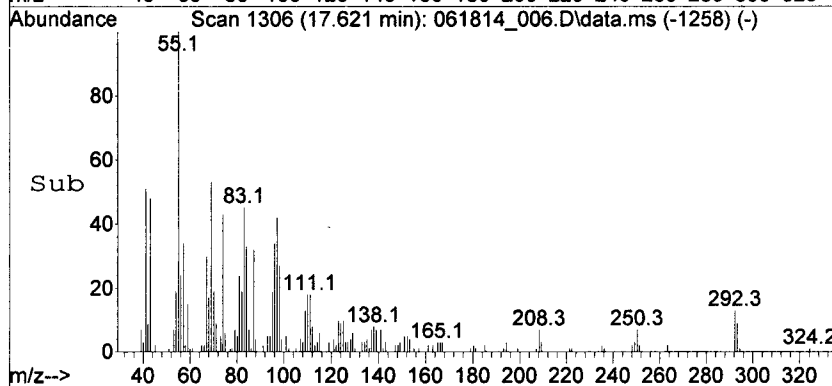
#33
Octadecanoic Acid-ME
Concen: N.D.
RT: 14.605 min Scan# 1015
Delta R.T. 0.003 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

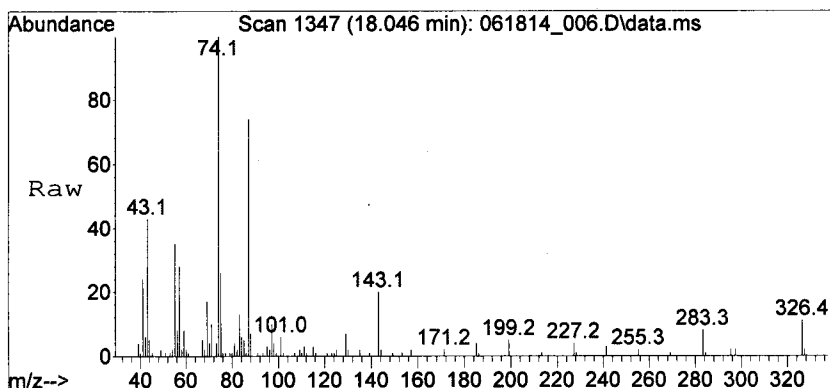
| | |
|-------------|----------------|
| Tgt Ion: 74 | Resp: 134400 |
| Ion Ratio | Lower Upper |
| 74 | 100 |
| 87 | 71.6 58.8 88.2 |
| 143 | 19.1 15.3 22.9 |



#34
cis-11-Eicosanoic Acid-ME
Concen: N.D. m
RT: 17.621 min Scan# 1306
Delta R.T. 0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

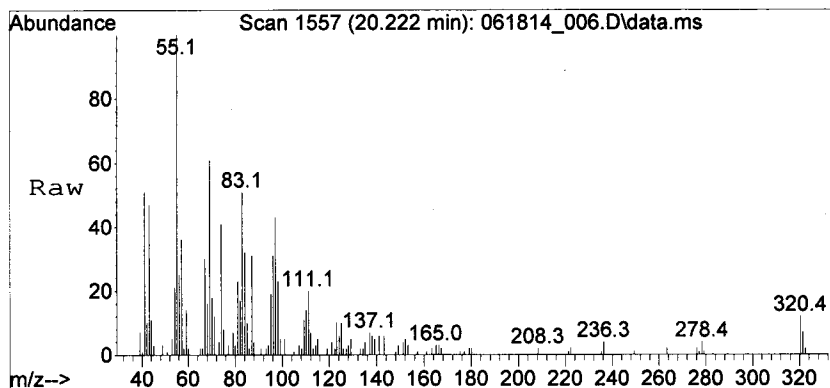
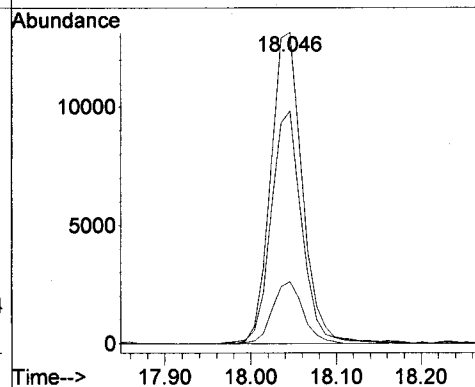
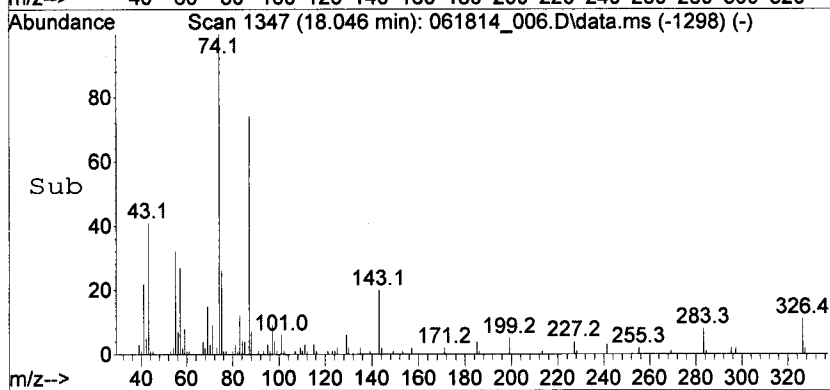
| | |
|-------------|----------------|
| Tgt Ion: 55 | Resp: 17178 |
| Ion Ratio | Lower Upper |
| 55 | 100 |
| 69 | 50.9 42.2 63.4 |
| 83 | 42.0 36.0 54.0 |





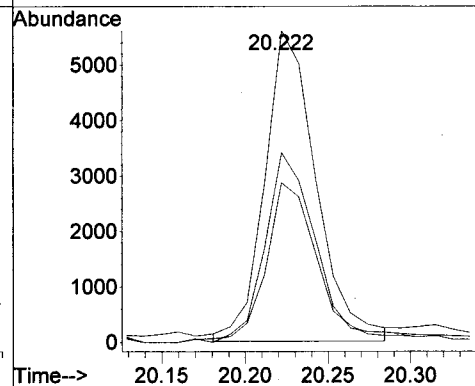
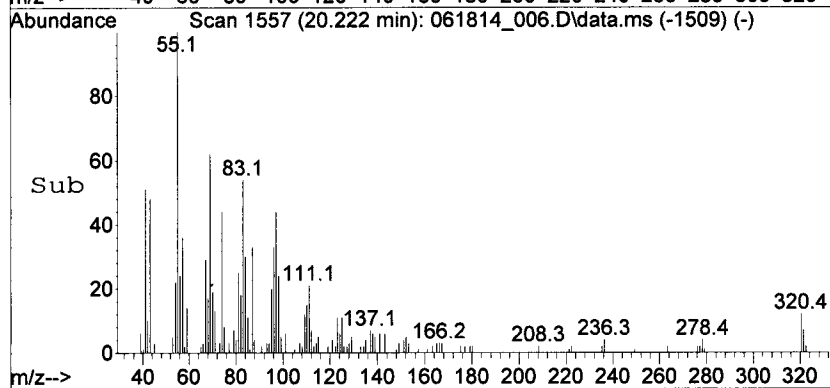
#35
Eicosanoic Acid-ME
Concen: N.D.
RT: 18.046 min Scan# 1347
Delta R.T. 0.003 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

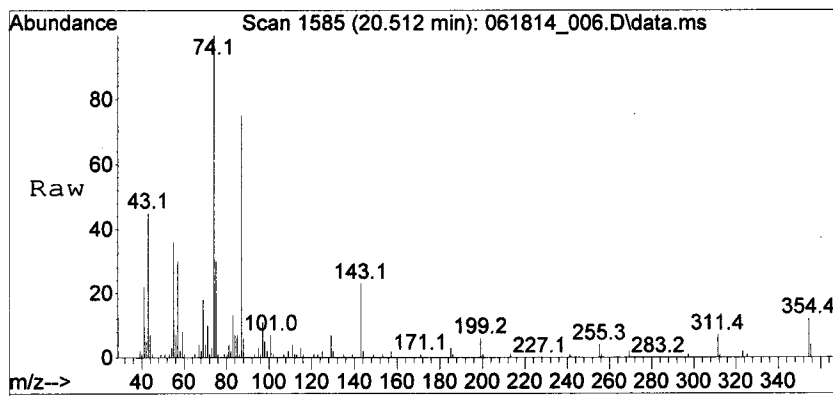
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 74 | 100 | | |
| 87 | 73.0 | 59.6 | 89.4 |
| 143 | 19.2 | 15.8 | 23.8 |



#36
Erucic Acid-ME
Concen: N.D. m
RT: 20.222 min Scan# 1557
Delta R.T. -0.002 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

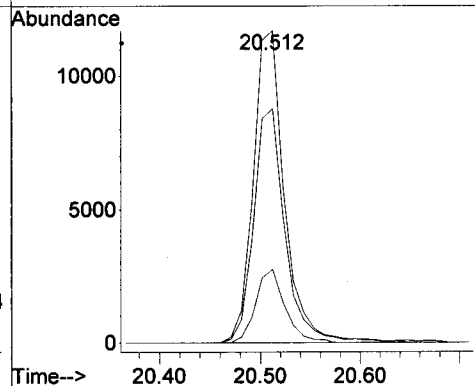
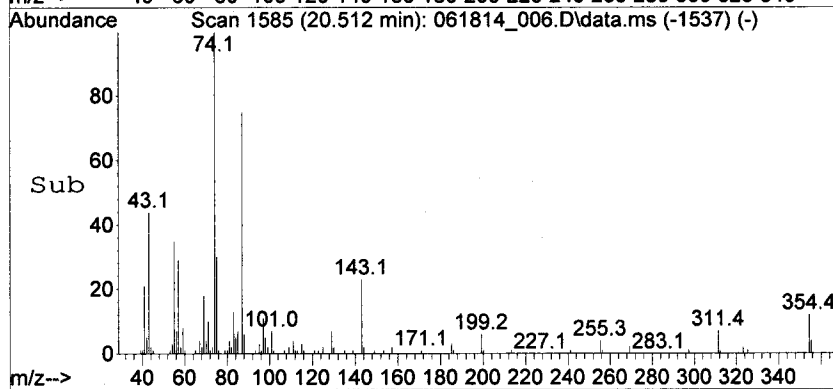
| Tgt Ion | Ratio | Lower | Upper |
|---------|-------|-------|-------|
| 55 | 100 | | |
| 69 | 64.5 | 48.8 | 73.2 |
| 83 | 54.0 | 41.0 | 61.6 |





#37
Docosanoic Acid-ME
Concen: N.D.
RT: 20.512 min Scan# 1585
Delta R.T. 0.001 min
Lab File: 061814_006.D
Acq: 18 Jun 2014 11:24 pm

| Tgt Ion | Ratio | Resp | Lower | Upper |
|---------|-------|-------|-------|-------|
| 74 | 100 | 25221 | | |
| 87 | 75.8 | 59.8 | 89.8 | |
| 143 | 22.1 | 18.7 | 28.1 | |



Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
Data File : 061814_007.D (C)
Acq On : 19 Jun 2014 12:00 am
Operator : (b) (7)(C)
Sample : Std Level 5-A
Misc : Calibration Standard 5
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Jun 19 16:12:45 2014
Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
Quant Title : RP1581 (b) (7)(C) Fatty Acids & MCHM
QLast Update : Thu Jun 19 10:44:37 2014
Response via : Initial Calibration

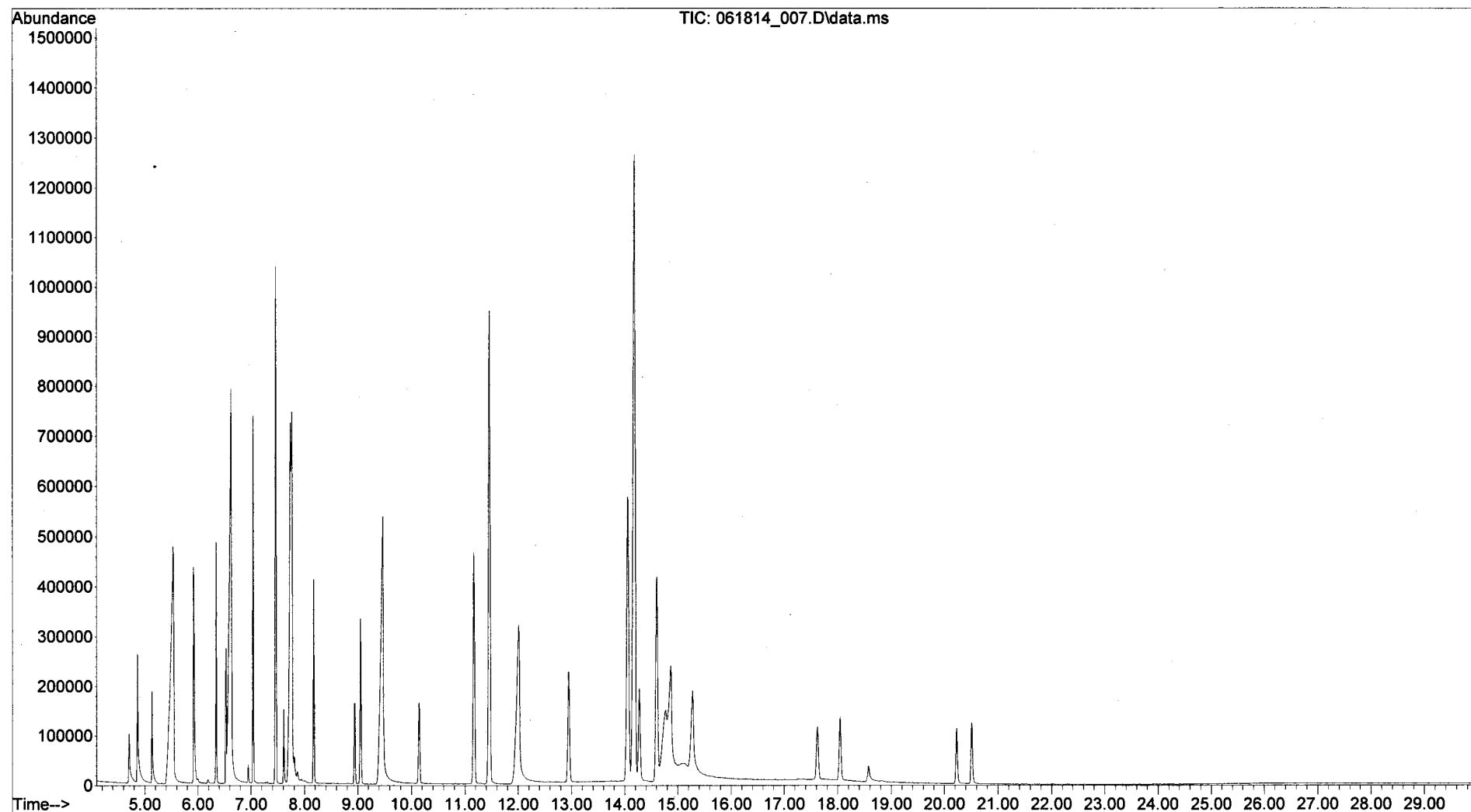
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) | |
|-------------------------------------|--------|------|----------|------|-------|-----------|--------|
| ----- | | | | | | | |
| Target Compounds | | | | | | | Qvalue |
| 1) Octanoic Acid | 5.538 | 60 | 436689 | No | Calib | | |
| 2) Decanoic Acid | 6.626 | 60 | 322167 | No | Calib | | |
| 3) Dodecanoic Acid | 7.766 | 60 | 277225 | No | Calib | | |
| 4) Tetradecanoic Acid | 9.476 | 60 | 197692 | No | Calib | | |
| 5) Hexadecanoic Acid | 12.015 | 73 | 131503 | No | Calib | | |
| 6) Linoleic Acid | 14.771 | 67 | 69226 | No | Calib | | |
| 7) Oleic Acid | 14.875 | 55 | 98193 | No | Calib | | |
| 8) Octadecanoic Acid | 15.279 | 60 | 49446 | No | Calib | | |
| 9) Eicosanoic Acid | 18.575 | 60 | 6759 | No | Calib | | |
| 10) MCHM (I) | 4.709 | 55 | 50528 | No | Calib | | # |
| 11) MCHM (II) | 4.864 | 55 | 108963 | No | Calib | | |
| 12) PPH | 5.921 | 94 | 191535 | No | Calib | | |
| 13) 1,4-CHDM (I) | 6.533 | 95 | 85308 | No | Calib | | |
| 14) 1,4-CHDM (II) | 6.636 | 95 | 29286 | No | Calib | | |
| 15) DMCH-1,4-DC | 7.040 | 81 | 108166 | No | Calib | | |
| 16) Di-PPH (I) | 7.610 | 59 | 36007 | No | Calib | | |
| 17) di-PPH (II) | 7.735 | 94 | 26410 | No | Calib | | |
| 18) di-PPH (III) | 7.807 | 94 | 2299 | No | Calib | | |
| 19) di-PPH (IV) | 7.869 | 94 | 1459 | No | Calib | | |
| 20) Octanoic Acid-ME | 5.134 | 74 | 58363 | No | Calib | | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 103405 | No | Calib | | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 208147 | No | Calib | | |
| 23) Tridecanoic Acid-ME | 8.170 | 74 | 103213 | No | Calib | | |
| 24) Myristolic Acid-ME | 8.937 | 55 | 28820 | No | Calib | | |
| 25) Tetradecanoic Acid-ME | 9.051 | 74 | 104754 | No | Calib | | |
| 26) Pentadecanoic Acid-ME | 10.139 | 74 | 61051 | No | Calib | | |
| 27) Palmitoleic Acid-ME PH. 7/25/14 | 11.165 | 55 | 85282 | No | Calib | | |
| 28) Hexadecanoic Acid-ME | 11.465 | 74 | 418546 | No | Calib | | |
| 29) Heptadecanoic Acid-ME | 12.947 | 74 | 99984 | No | Calib | | |
| 30) Linoleic Acid-ME | 14.056 | 67 | 142337 | No | Calib | | |
| 31) Linolenic/Oleic Acid-MES | 14.191 | 55 | 283239 | No | Calib | | |
| 32) Elaidic Acid-ME | 14.274 | 55 | 39015 | No | Calib | | |
| 33) Octadecanoic Acid-ME | 14.605 | 74 | 206297 | No | Calib | | |
| 34) cis-11-Eicosanoic Acid-ME | 17.621 | 55 | 30044 | No | Calib | | |
| 35) Eicosanoic Acid-ME | 18.046 | 74 | 55065 | No | Calib | | |
| 36) Erucic Acid-ME | 20.233 | 55 | 21890 | No | Calib | | |
| 37) Docosanoic Acid-ME | 20.512 | 74 | 42879 | No | Calib | | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
 Data File : 061814_007.D (C)
 Acq On : 19 Jun 2014 12:00 am
 Operator : (b) (7)(C)
 Sample : Std Level 5-A
 Misc : Calibration Standard 5
 ALS Vial : 7 Sample Multiplier: 1

Quant Time: Jun 19 16:12:45 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



Data Path : D:\RP1581 (b) (7) 061314 (b) (7) 061814 Run\
Data File : 061814_008.D
Acq On : 19 Jun 2014 12:36 am
Operator : (b) (7)(C)
Sample : Std Level 6-A
Misc : Calibration Standard 6
ALS Vial : 8 Sample Multiplier: 1

Quant Time: Jun 19 11:54:32 2014
Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
QLast Update : Thu Jun 19 10:44:37 2014
Response via : Initial Calibration

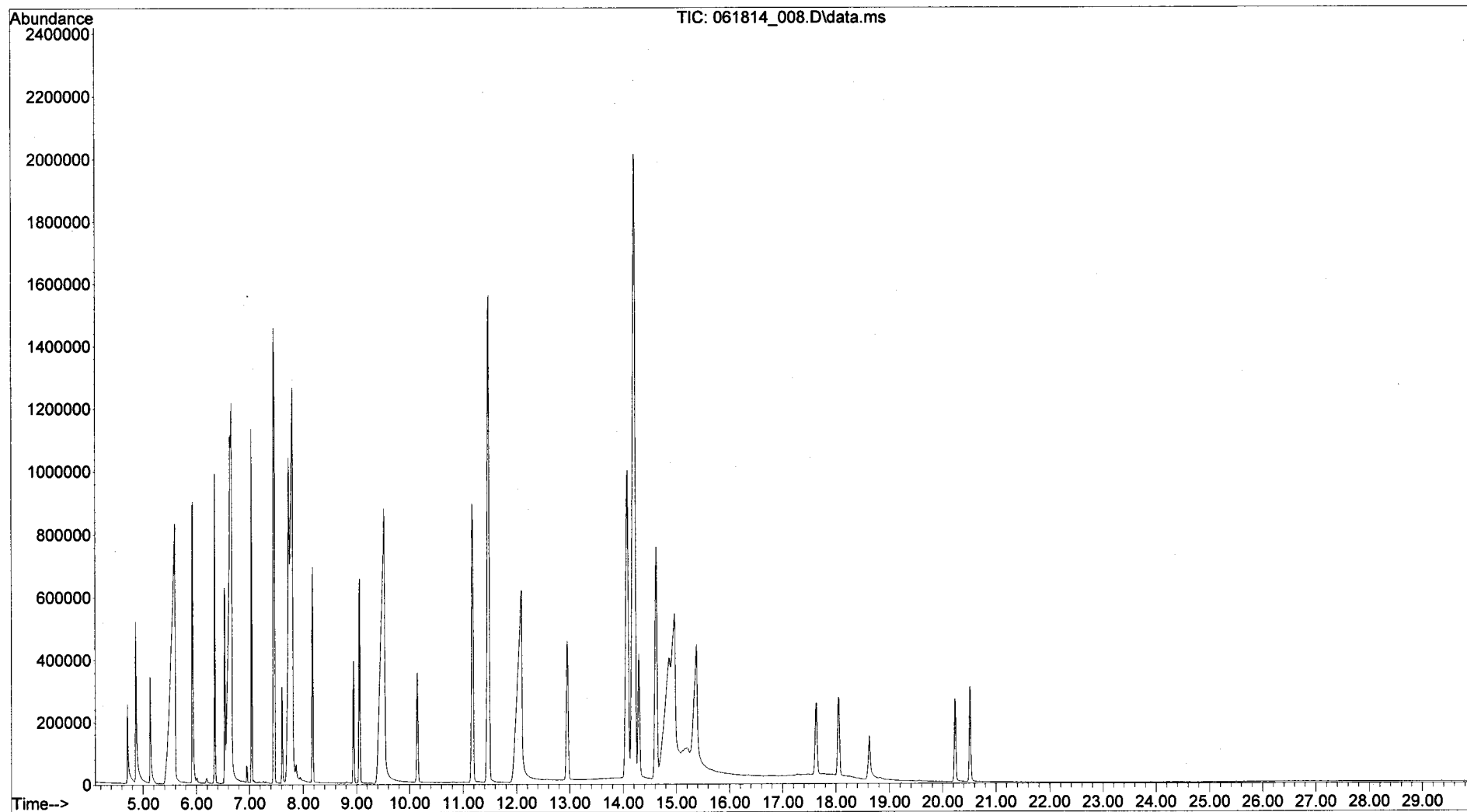
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) | |
|---|--------|------|----------|------|-------|-----------|--------|
| ----- | | | | | | | |
| Target Compounds | | | | | | | Qvalue |
| 1) Octanoic Acid | 5.600 | 60 | 922605 | No | Calib | | |
| 2) Decanoic Acid | 6.667 | 60 | 678496 | No | Calib | | |
| 3) Dodecanoic Acid | 7.807 | 60 | 587121 | No | Calib | | |
| 4) Tetradecanoic Acid | 9.527 | 60 | 445474 | No | Calib | | |
| 5) Hexadecanoic Acid | 12.097 | 73 | 341157 | No | Calib | | |
| 6) Linoleic Acid | 14.864 | 67 | 236501 | No | Calib | | |
| 7) Oleic Acid | 14.968 | 55 | 245188 | No | Calib | | |
| 8) Octadecanoic Acid | 15.382 | 60 | 146106 | No | Calib | | |
| 9) Eicosanoic Acid | 18.626 | 60 | 30835 | No | Calib | | |
| 10) MCHM (I) | 4.709 | 55 | 106376 | No | Calib | | |
| 11) MCHM (II) | 4.864 | 55 | 212269 | No | Calib | | |
| 12) PPH | 5.931 | 94 | 383473 | No | Calib | | |
| 13) 1,4-CHDM (I) | 6.532 | 95 | 166492 | No | Calib | | |
| 14) 1,4-CHDM (II) | 6.636 | 95 | 59129 | No | Calib | | |
| 15) DMCH-1,4-DC | 7.040 | 81 | 203191 | No | Calib | | |
| 16) Di-PPH (I) | 7.610 | 59 | 77931 | No | Calib | | |
| 17) di-PPH (II) | 7.735 | 94 | 51800 | No | Calib | | |
| 18) di-PPH (III) | 7.807 | 94 | 5611 | No | Calib | | |
| 19) di-PPH (IV) | 7.869 | 94 | 2695 | No | Calib | | |
| 20) Octanoic Acid-ME | 5.133 | 74 | 116120 | No | Calib | | |
| 21) Decanoic Acid-ME | 6.346 | 74 | 209319 | No | Calib | | |
| 22) Dodecanoic Acid-ME | 7.465 | 74 | 391150 | No | Calib | | # |
| 23) Tridecanoic Acid-ME | 8.180 | 74 | 206449 | No | Calib | | |
| 24) Myristolic Acid-ME | 8.947 | 55 | 60326 | No | Calib | | |
| 25) Tetradecanoic Acid-ME | 9.061 | 74 | 211896 | No | Calib | | |
| 26) Pentadecanoic Acid-ME | 10.149 | 74 | 125550 | No | Calib | | |
| 27) Palmitoleic Acid-ME (b) (7) 7/25/14 | 11.175 | 55 | 174274 | No | Calib | | |
| 28) Hexadecanoic Acid-ME (b) (7) | 11.486 | 74 | 817153 | No | Calib | | |
| 29) Heptadecanoic Acid-ME | 12.958 | 74 | 207034 | No | Calib | | |
| 30) Linoleic Acid-ME | 14.087 | 67 | 290518 | No | Calib | | |
| 31) Linolenic/Oleic Acid-MEs | 14.222 | 55 | 544302 | No | Calib | | |
| 32) Elaidic Acid-ME | 14.294 | 55 | 81076 | No | Calib | | |
| 33) Octadecanoic Acid-ME | 14.626 | 74 | 407250 | No | Calib | | |
| 34) cis-11-Eicosanoic Acid-ME | 17.631 | 55 | 63310 | No | Calib | | |
| 35) Eicosanoic Acid-ME | 18.056 | 74 | 115364 | No | Calib | | |
| 36) Erucic Acid-ME | 20.232 | 55 | 49848 | No | Calib | | |
| 37) Docosanoic Acid-ME | 20.512 | 74 | 96381 | No | Calib | | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data Path : D:\RP1581\ (b) (7) 061314\ (b) (7) 061814 Run\
 Data File : 061814_008.D (b) (7) (C)
 Acq On : 19 Jun 2014 12:36 am
 Operator : (b) (7) (C)
 Sample : Std Level 6-A
 Misc : Calibration Standard 6
 ALS Vial : 8 Sample Multiplier: 1

Quant Time: Jun 19 11:54:32 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) RP1581_Fatty Acids.M
 Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



Data Path : D:\RP1581\ (b) (7) 061314 (b) (7) 061814 Run\
Data File : 061814_009.D (C)
Acq On : 19 Jun 2014 1:12 am
Operator : (b) (7)(C)
Sample : CH2Cl2 Blank
Misc : Injection Blank
ALS Vial : 9 Sample Multiplier: 1

Quant Time: Jun 19 12:09:04 2014
Quant Method : C:\msdchem\1\METHODS (b) (7)(C) P1581_Fatty Acids.M
Quant Title : RP1581 (b) (7) Fatty Acids & MCHM
QLast Update : Thu Jun 19 10:44:37 2014
Response via : Initial Calibration

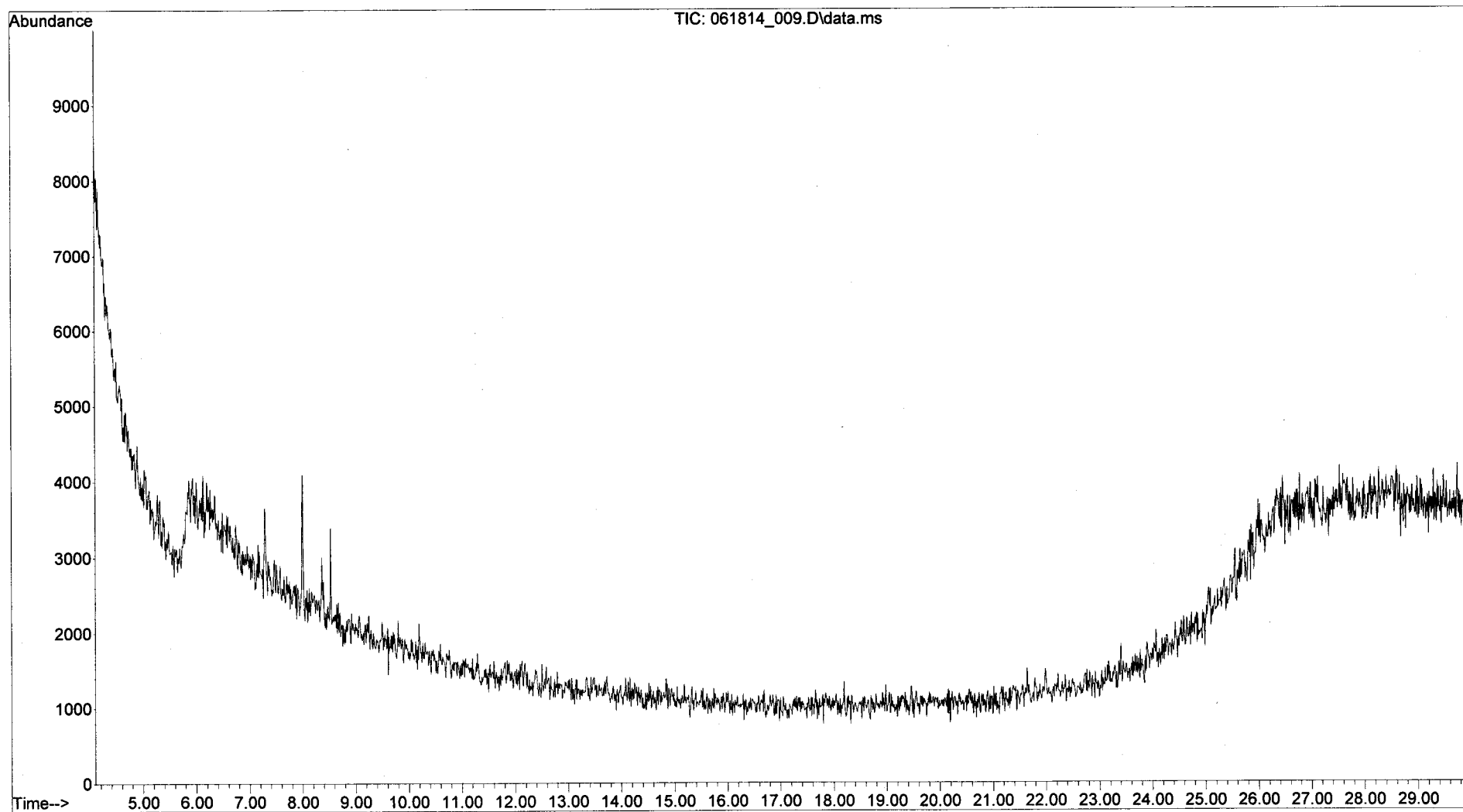
| Compound | R.T. | QIon | Response | Conc | Units | Dev (Min) |
|--|-------|------|----------|------|-------|-----------|
| ----- | | | | | | |
| Target Compounds | | | | | | Qvalue |
| 1) Octanoic Acid | 0.000 | | 0 | N.D. | | |
| 2) Decanoic Acid | 0.000 | | 0 | N.D. | | |
| 3) Dodecanoic Acid | 0.000 | | 0 | N.D. | | |
| 4) Tetradecanoic Acid | 0.000 | | 0 | N.D. | | |
| 5) Hexadecanoic Acid | 0.000 | | 0 | N.D. | d | |
| 6) Linoleic Acid | 0.000 | | 0 | N.D. | | |
| 7) Oleic Acid | 0.000 | | 0 | N.D. | d | |
| 8) Octadecanoic Acid | 0.000 | | 0 | N.D. | | |
| 9) Eicosanoic Acid | 0.000 | | 0 | N.D. | | |
| 10) MCHM (I) | 0.000 | | 0 | N.D. | d | |
| 11) MCHM (II) | 0.000 | | 0 | N.D. | d | |
| 12) PPH | 0.000 | | 0 | N.D. | | |
| 13) 1,4-CHDM (I) | 0.000 | | 0 | N.D. | | |
| 14) 1,4-CHDM (II) | 0.000 | | 0 | N.D. | | |
| 15) DMCH-1,4-DC | 0.000 | | 0 | N.D. | | |
| 16) Di-PPH (I) | 0.000 | | 0 | N.D. | | |
| 17) di-PPH (II) | 0.000 | | 0 | N.D. | | |
| 18) di-PPH (III) | 0.000 | | 0 | N.D. | | |
| 19) di-PPH (IV) | 0.000 | | 0 | N.D. | | |
| 20) Octanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 21) Decanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 22) Dodecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 23) Tridecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 24) Myristolic Acid-ME | 0.000 | | 0 | N.D. | d | |
| 25) Tetradecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 26) Pentadecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 27) Palmitoleic Acid-ME <i>DN. 7/27/14</i> | 0.000 | | 0 | N.D. | d | |
| 28) Hexadecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 29) Heptadecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 30) Linoleic Acid-ME | 0.000 | | 0 | N.D. | | |
| 31) Linolenic/Oleic Acid-MEs | 0.000 | | 0 | N.D. | d | |
| 32) Elaidic Acid-ME | 0.000 | | 0 | N.D. | d | |
| 33) Octadecanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 34) cis-11-Eicosanoic Acid-ME | 0.000 | | 0 | N.D. | d | |
| 35) Eicosanoic Acid-ME | 0.000 | | 0 | N.D. | | |
| 36) Erucic Acid-ME | 0.000 | | 0 | N.D. | d | |
| 37) Docosanoic Acid-ME | 0.000 | | 0 | N.D. | | |

(#) = qualifier out of range (m) = manual integration (+) = signals summed

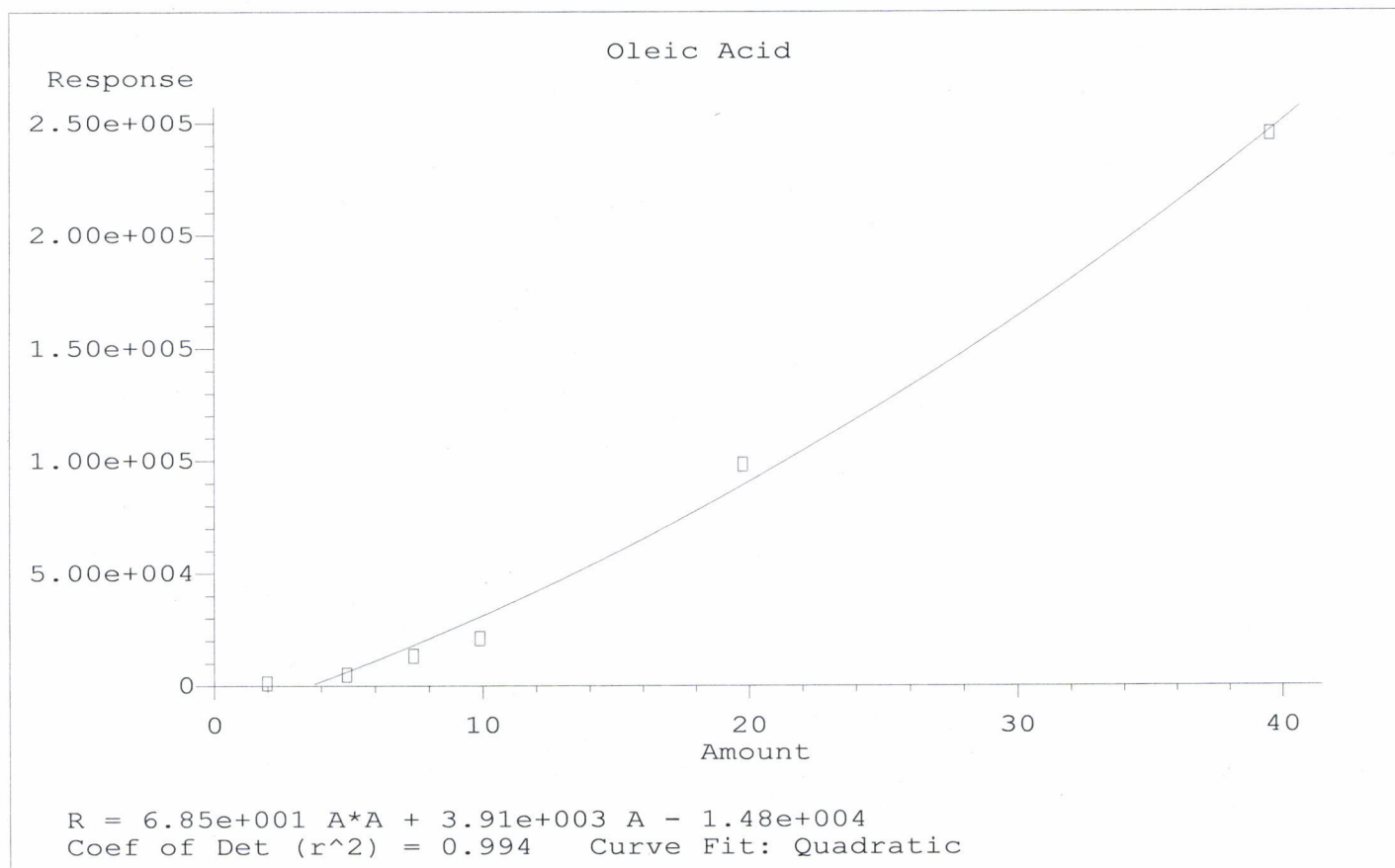
Quantitation Report (QT Reviewed)

Data Path : D:\RP1581\ (b) (7) (C) 061314\ (b) (7) (C) 061814 Run\
 Data File : 061814_009.D
 Acq On : 19 Jun 2014 1:12 am
 Operator : (b) (7) (C)
 Sample : CH2Cl2 Blank
 Misc : Injection Blank
 ALS Vial : 9 Sample Multiplier: 1

Quant Time: Jun 19 12:09:04 2014
 Quant Method : C:\msdchem\1\METHODS (b) (7) (C) RP1581_Fatty Acids.M
 Quant Title : RP158 (b) (7) (C) Fatty Acids & MCHM
 QLast Update : Thu Jun 19 10:44:37 2014
 Response via : Initial Calibration



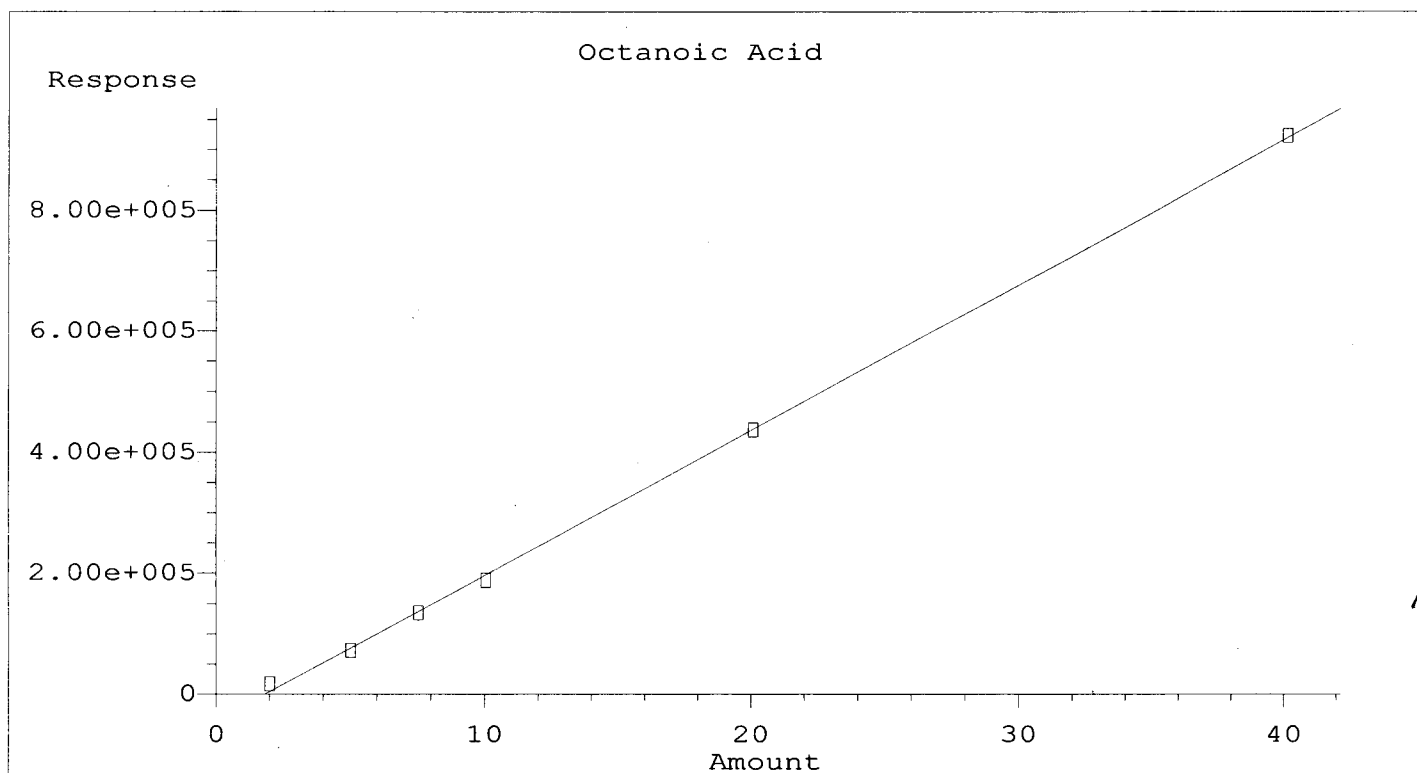
Calibration Plot Report



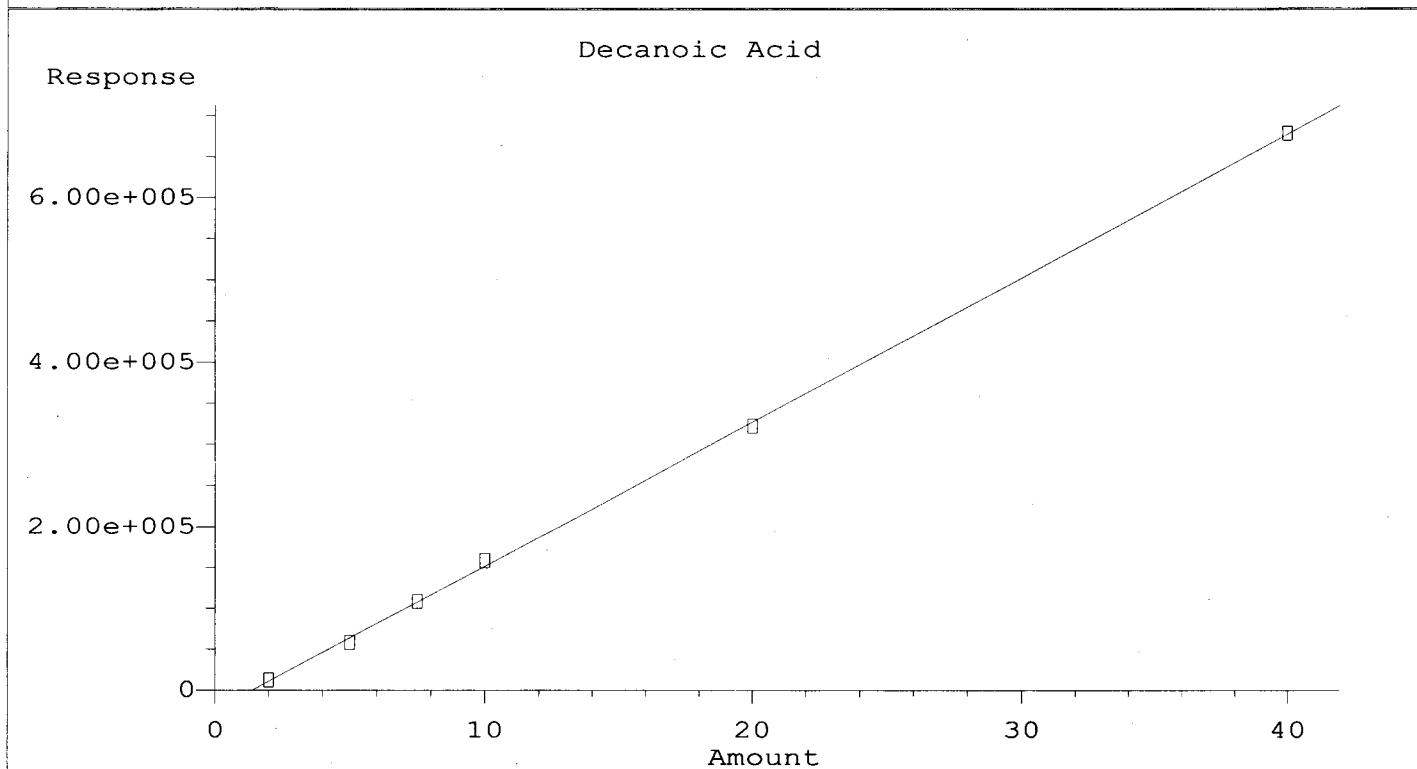
w/ [oleic] in Cal Std 1 = $1.98 \frac{\mu\text{g}}{\text{mL}}$

(b) (7)
(C) 5/3/14

Calibration Plot Report

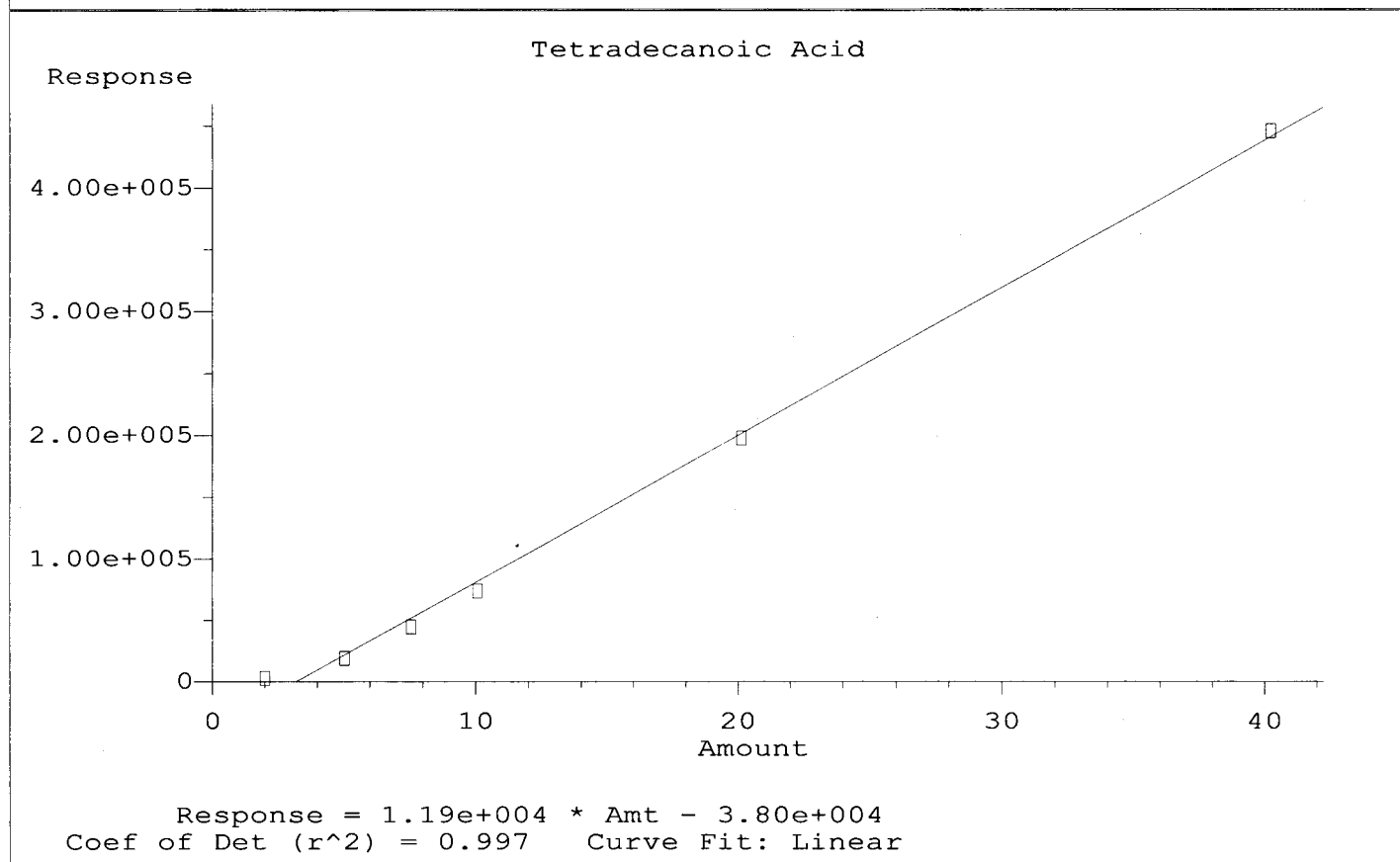
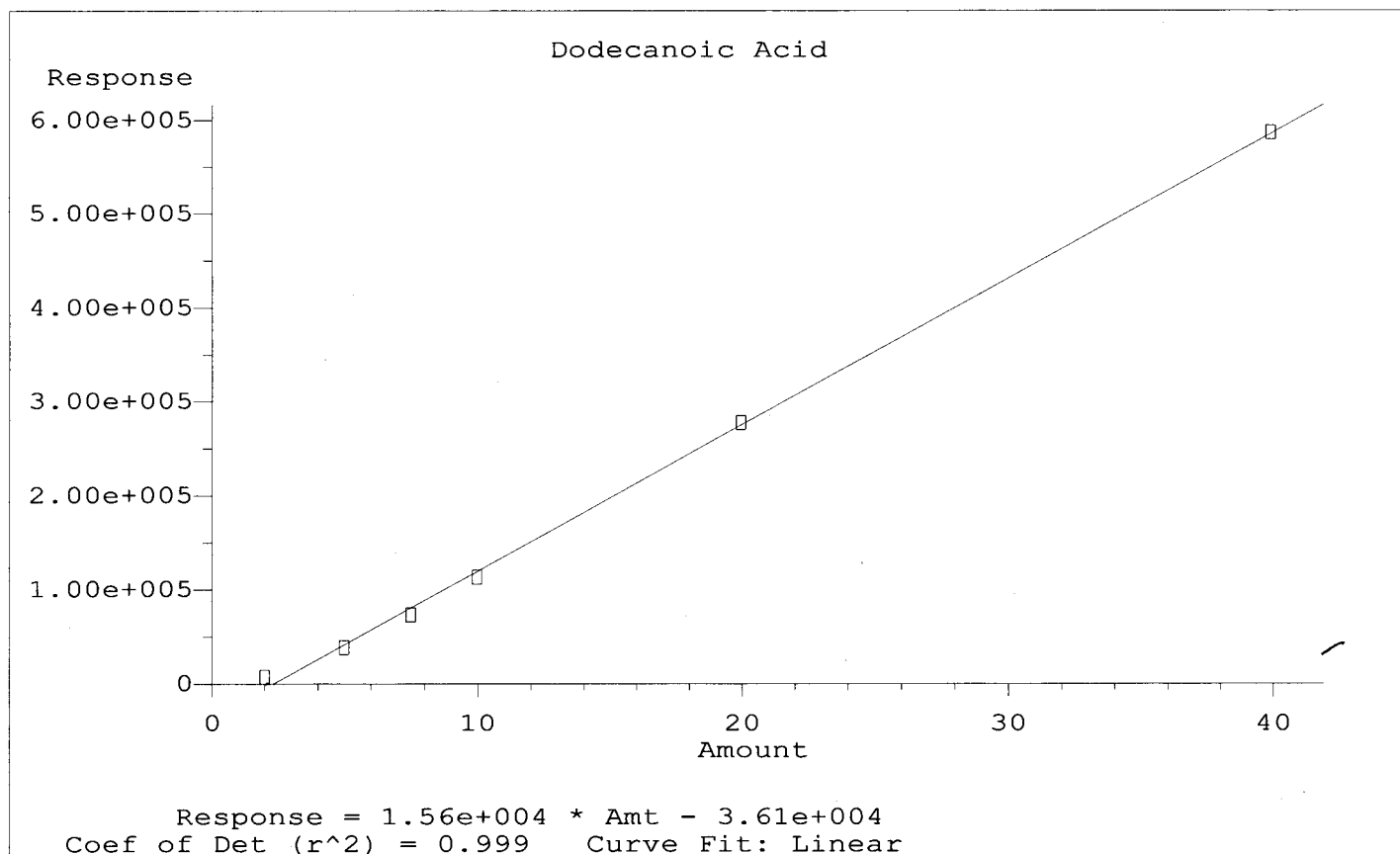


Response = 2.40×10^4 * Amt - 4.39×10^4
Coef of Det (r^2) = 1.000 Curve Fit: Linear

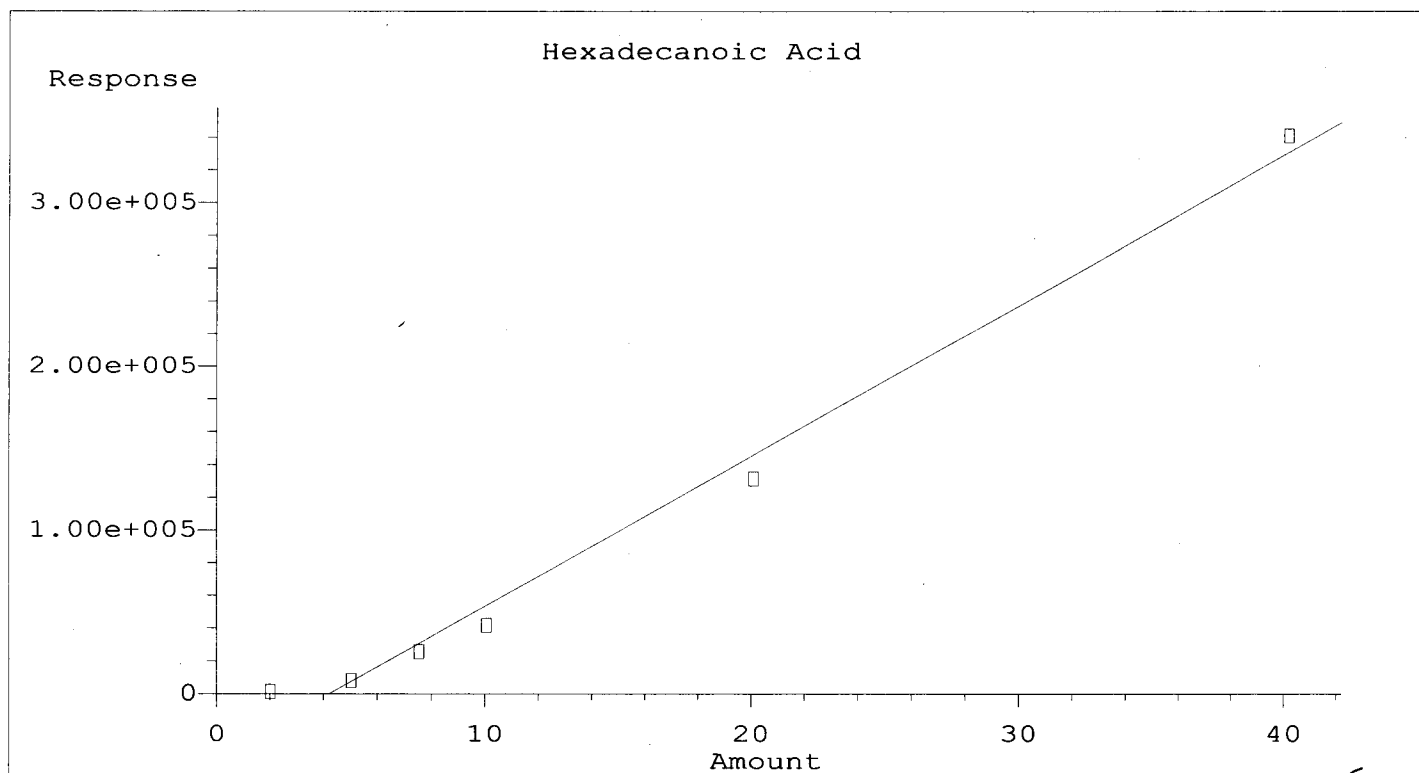


Response = 1.76×10^4 * Amt - 2.40×10^4
Coef of Det (r^2) = 1.000 Curve Fit: Linear

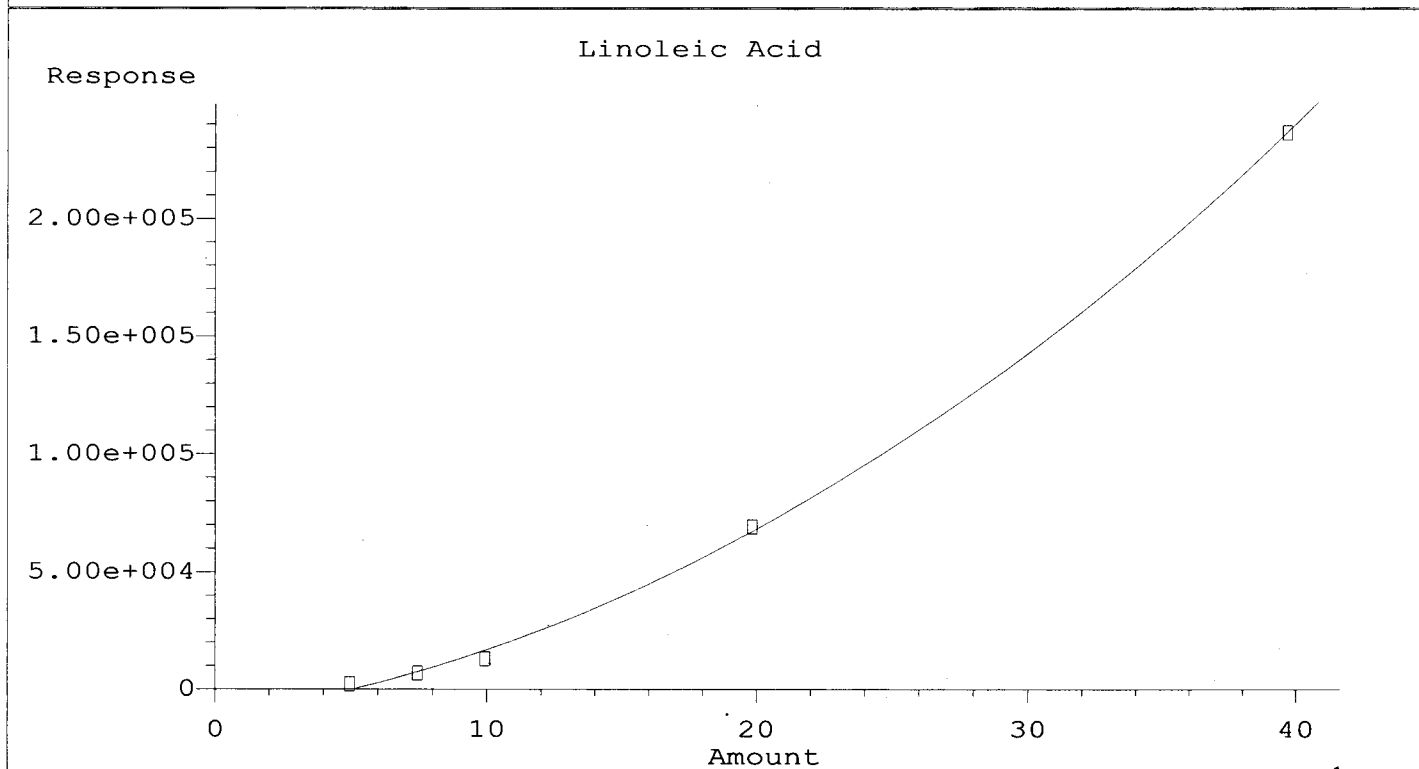
Calibration Plot Report



Calibration Plot Report

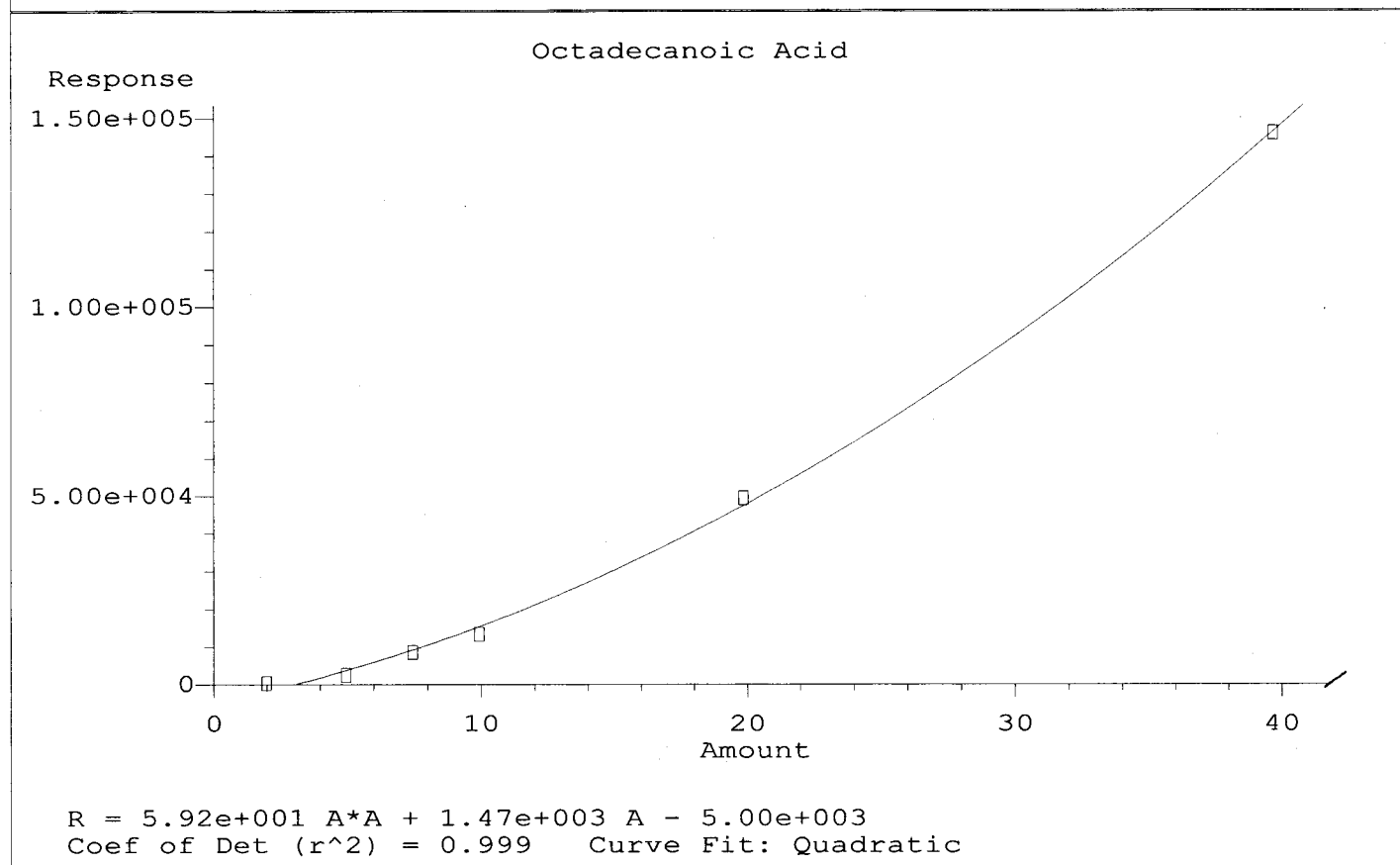
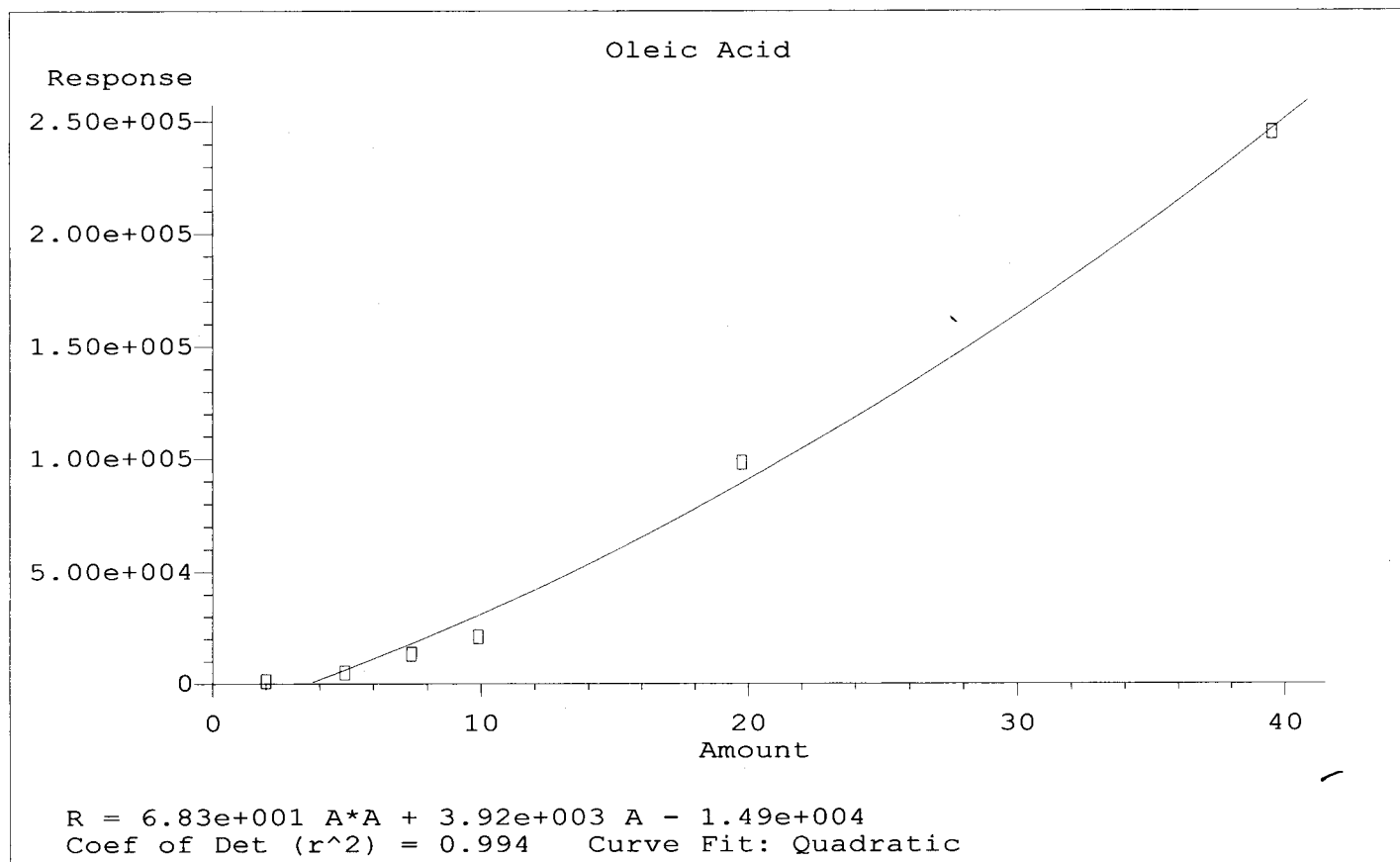


Response = $9.19e+003 \cdot \text{Amt} - 3.86e+004$
 Coef of Det (r^2) = 0.989 Curve Fit: Linear

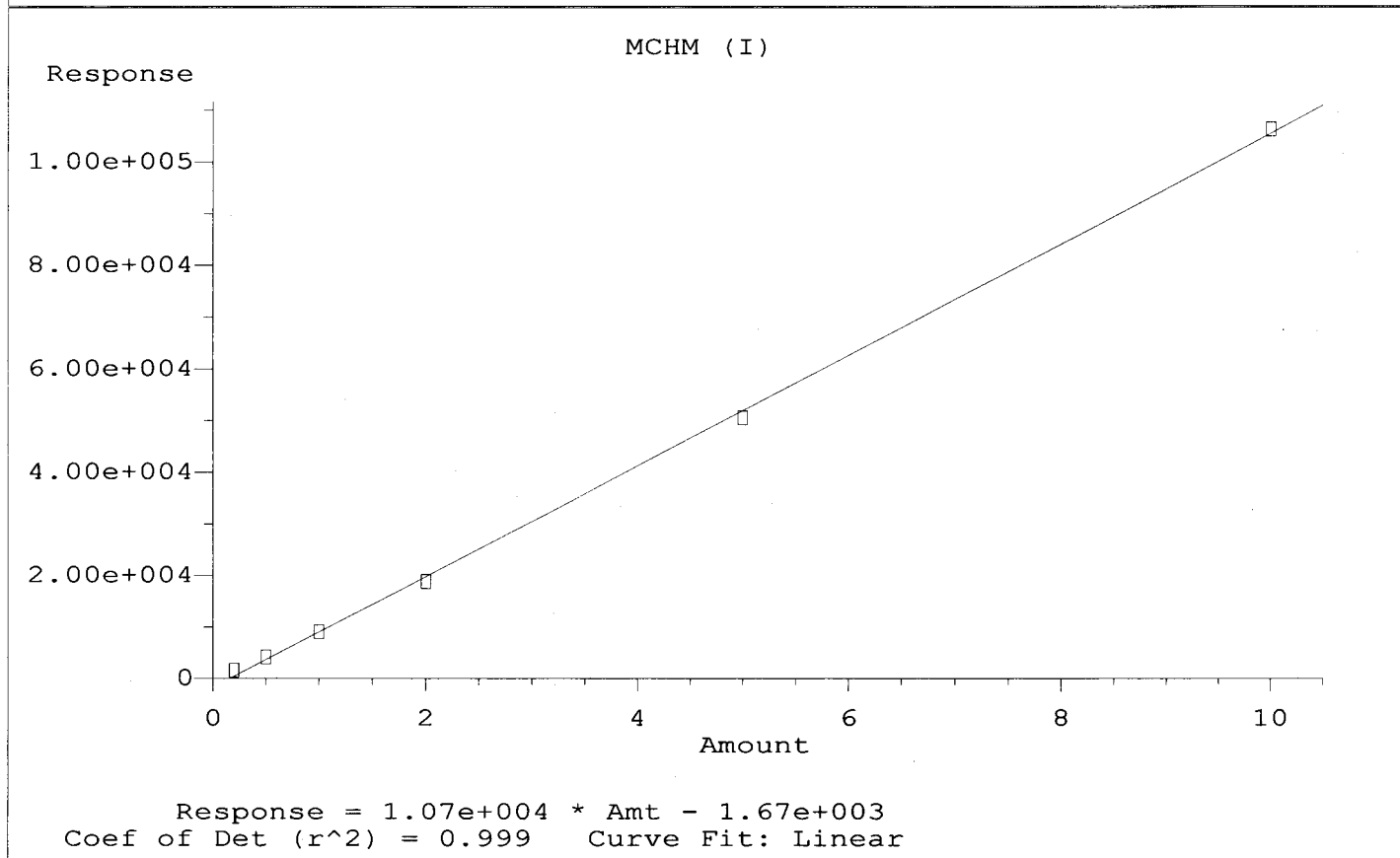
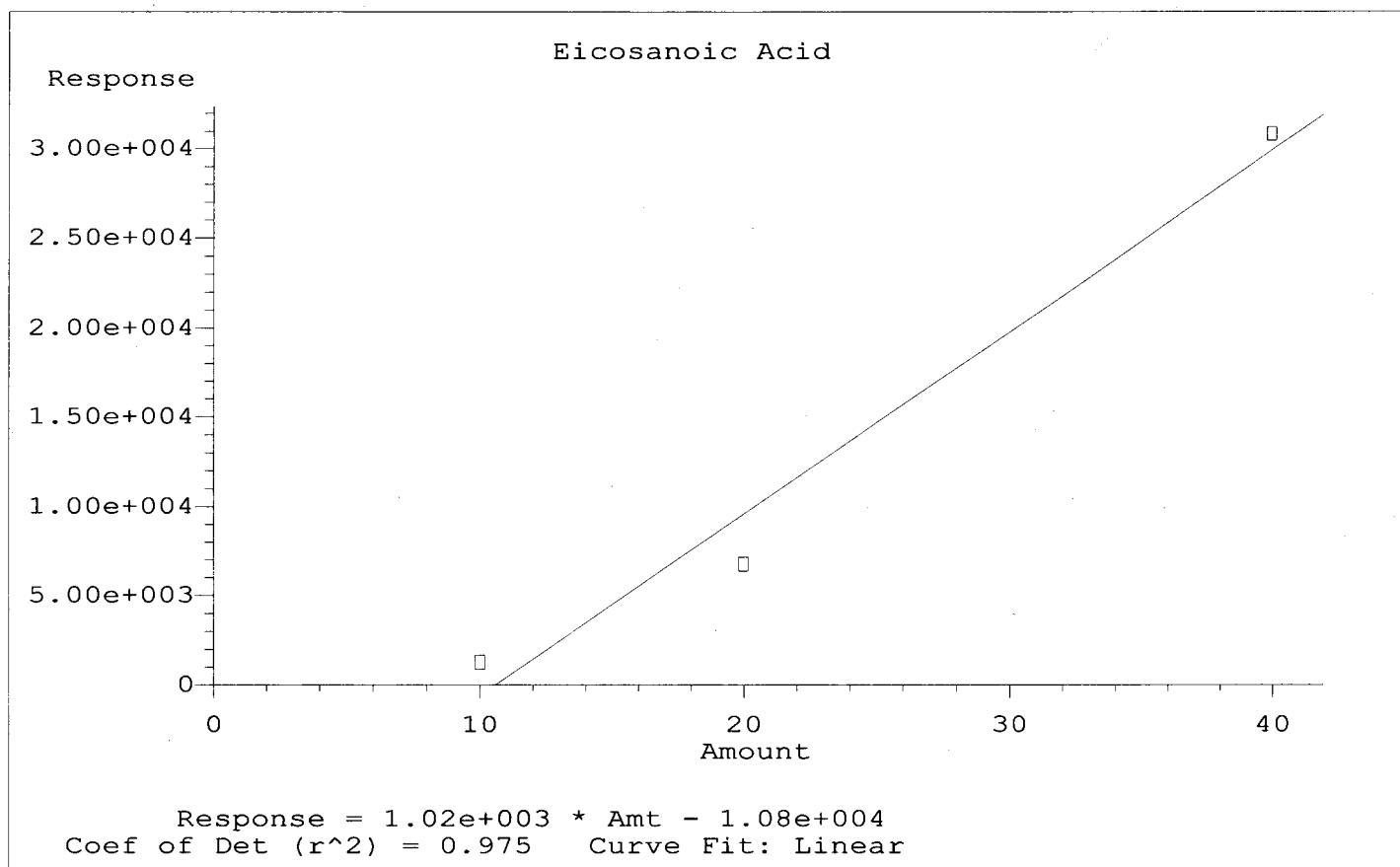


$R = 1.15e+002 A^2 + 1.68e+003 A - 1.15e+004$
 Coef of Det (r^2) = 0.999 Curve Fit: Quadratic

Calibration Plot Report



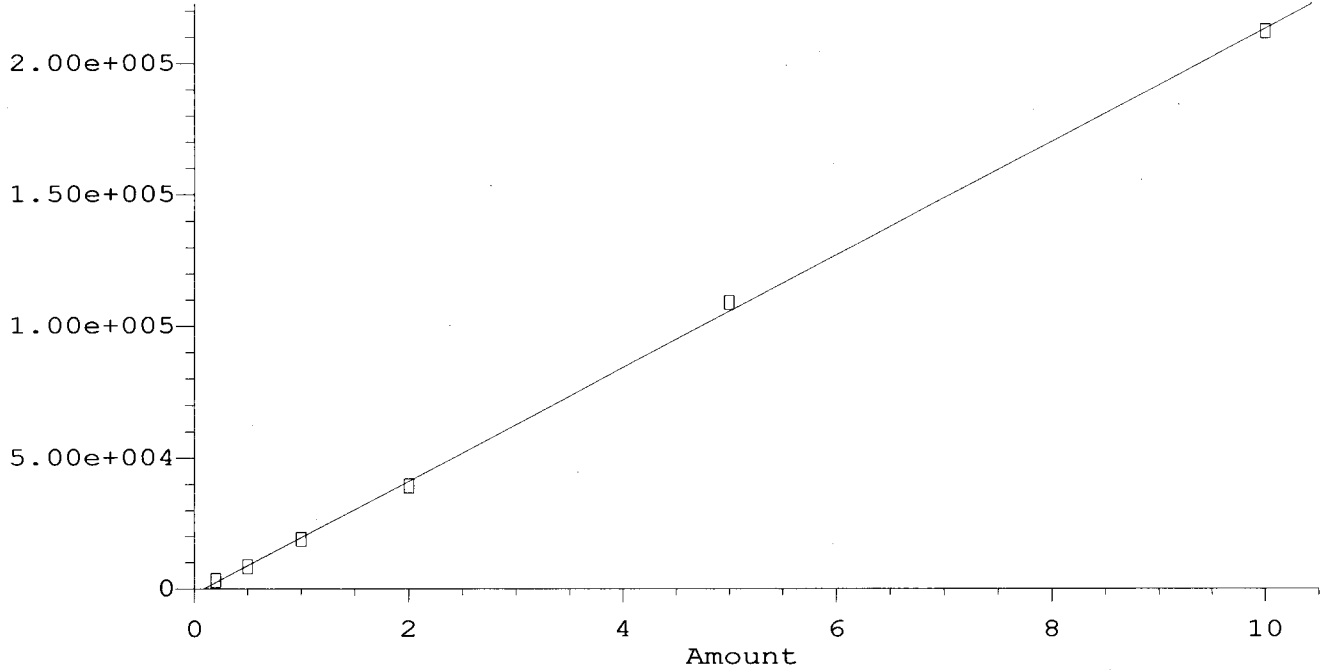
Calibration Plot Report



Calibration Plot Report

Response

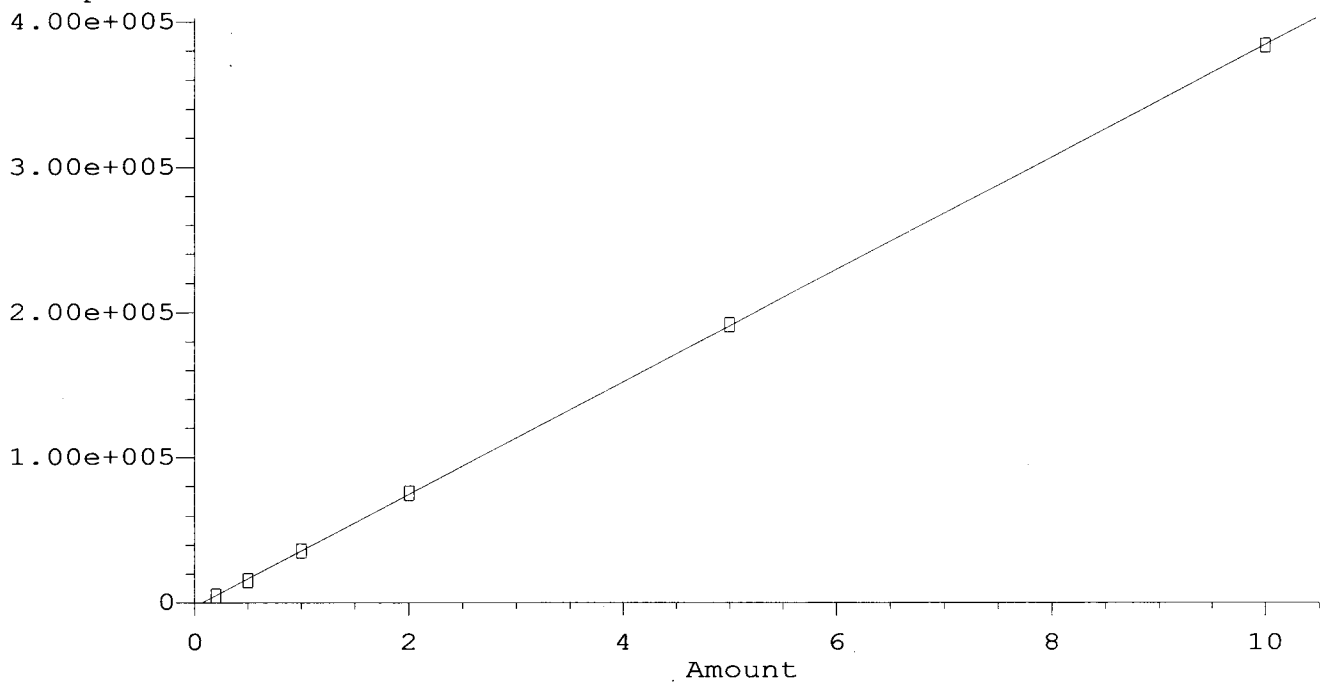
MCHM (II)



Response = $2.15e+004 * \text{Amt} - 1.98e+003$
Coef of Det (r^2) = 1.000 Curve Fit: Linear

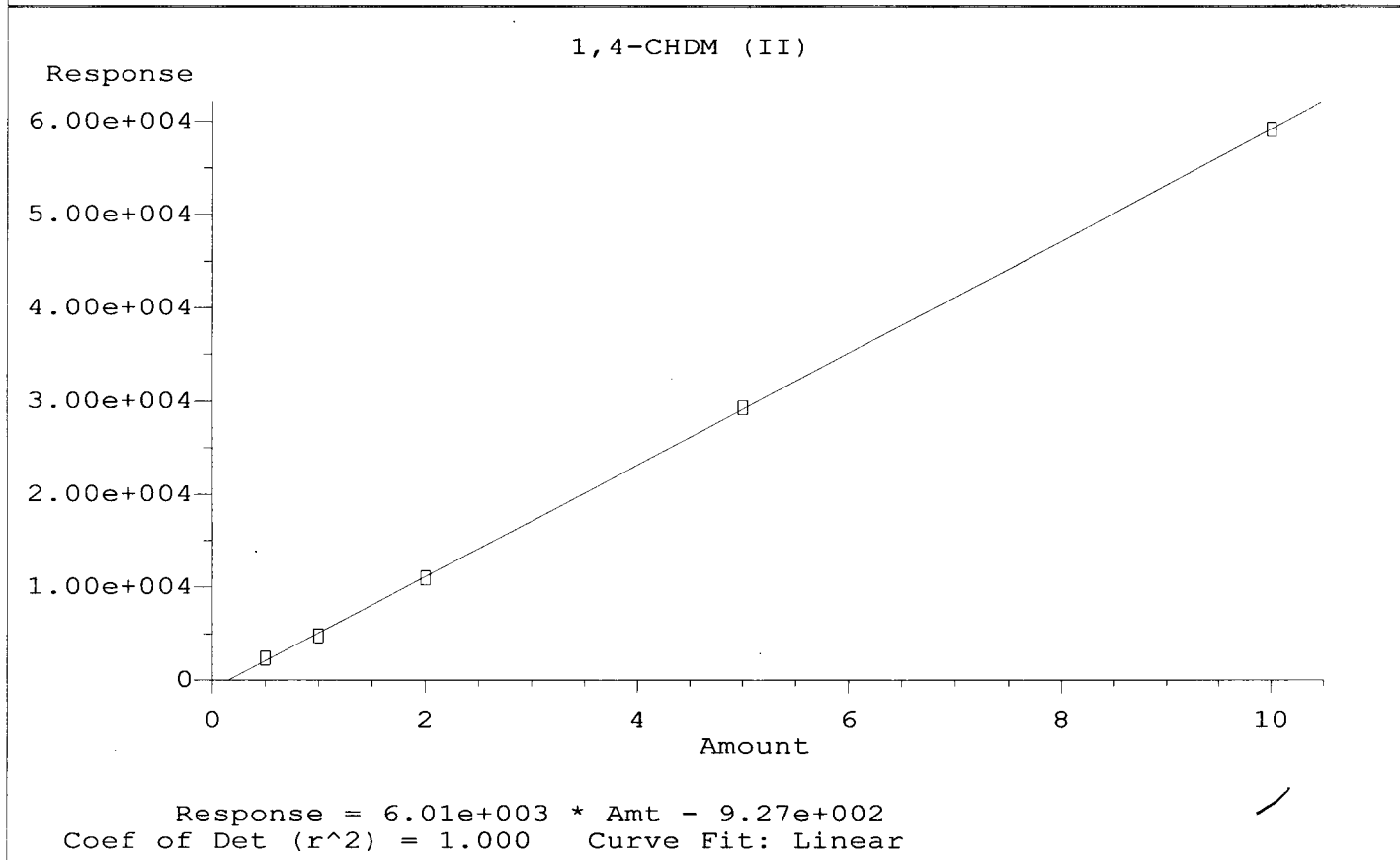
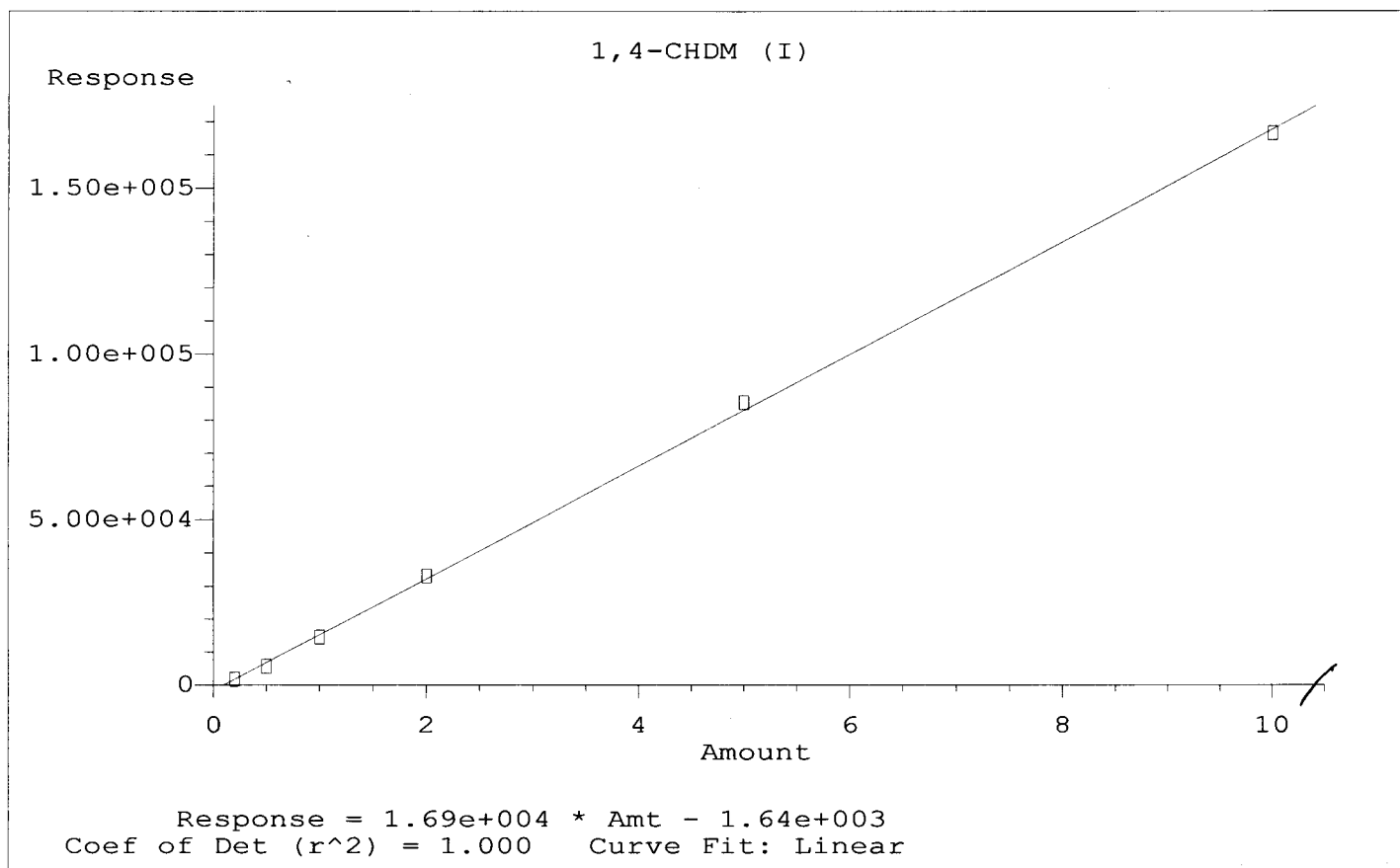
Response

PPH

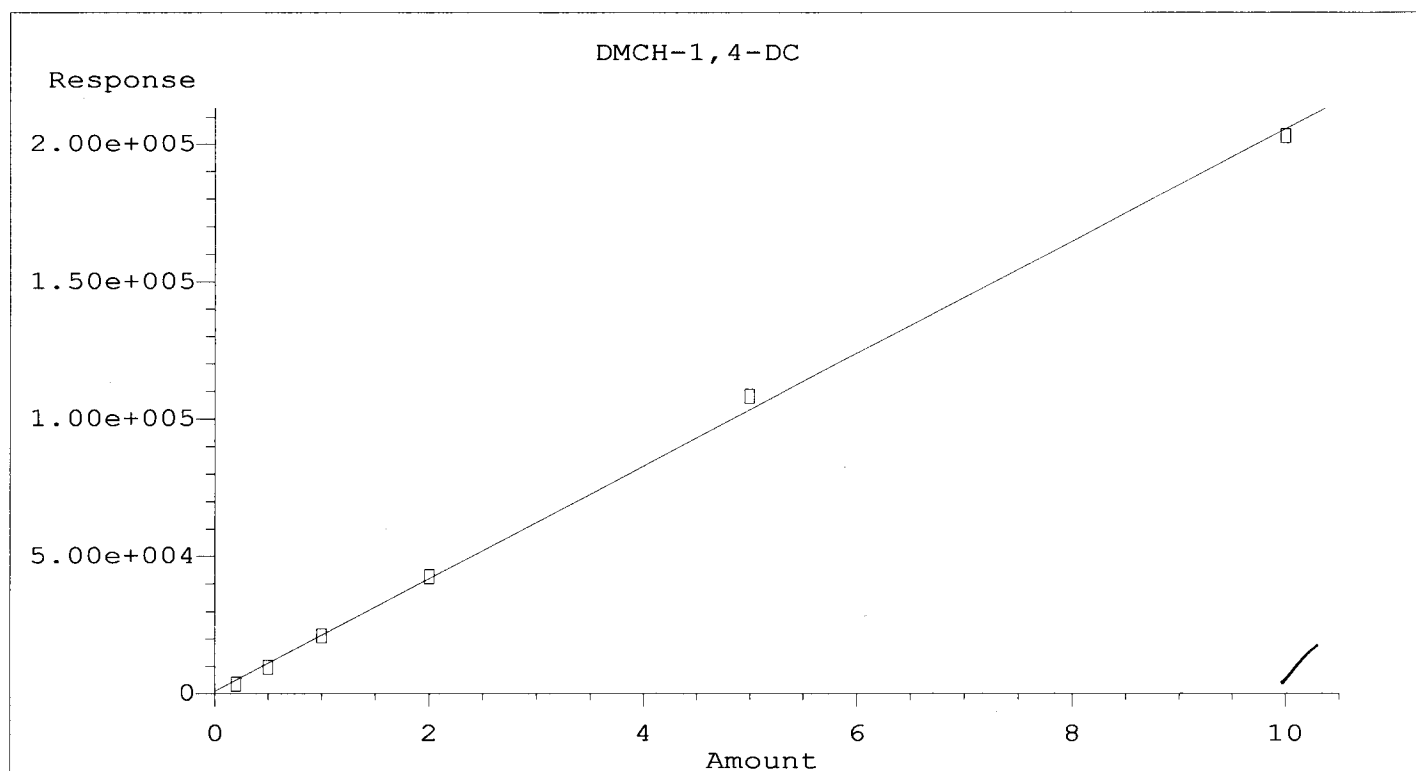


Response = $3.87e+004 * \text{Amt} - 2.75e+003$
Coef of Det (r^2) = 1.000 Curve Fit: Linear

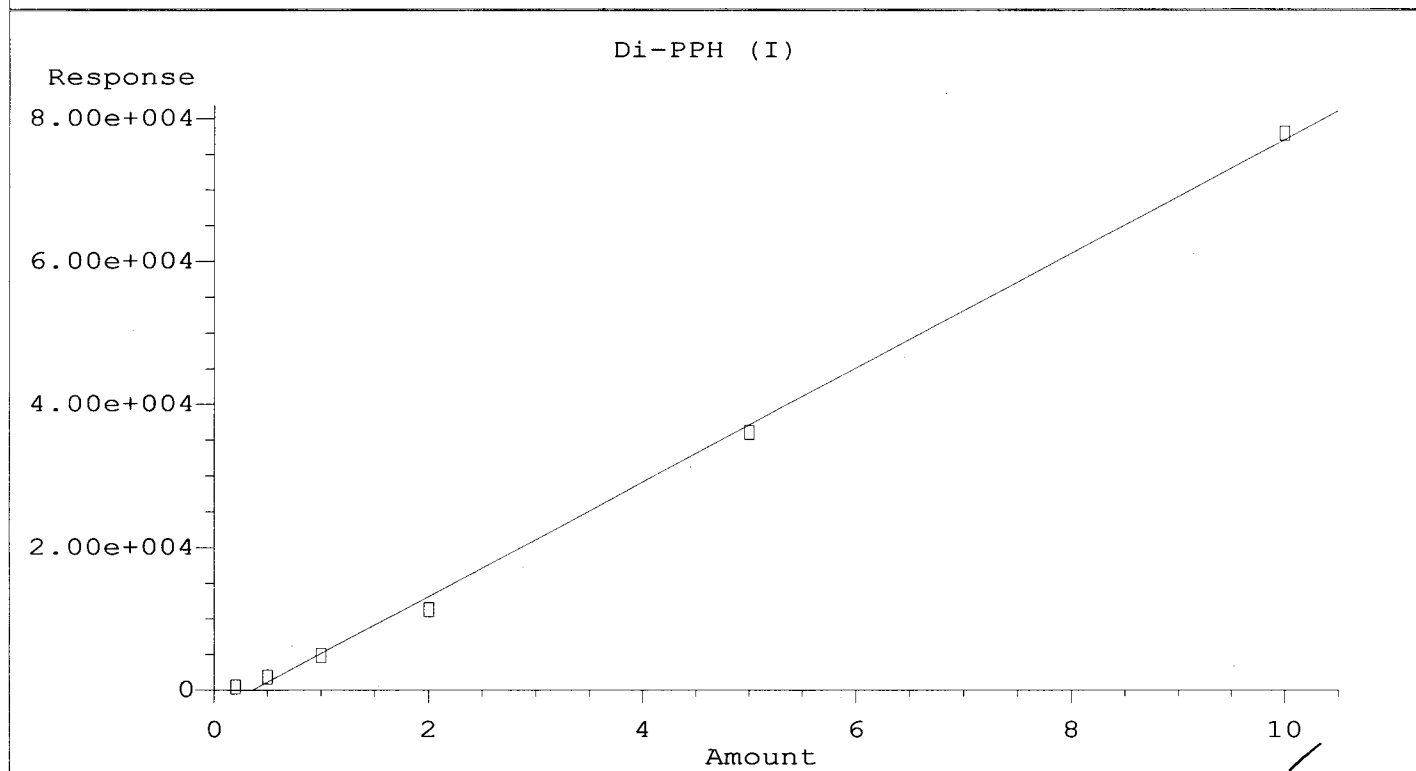
Calibration Plot Report



Calibration Plot Report

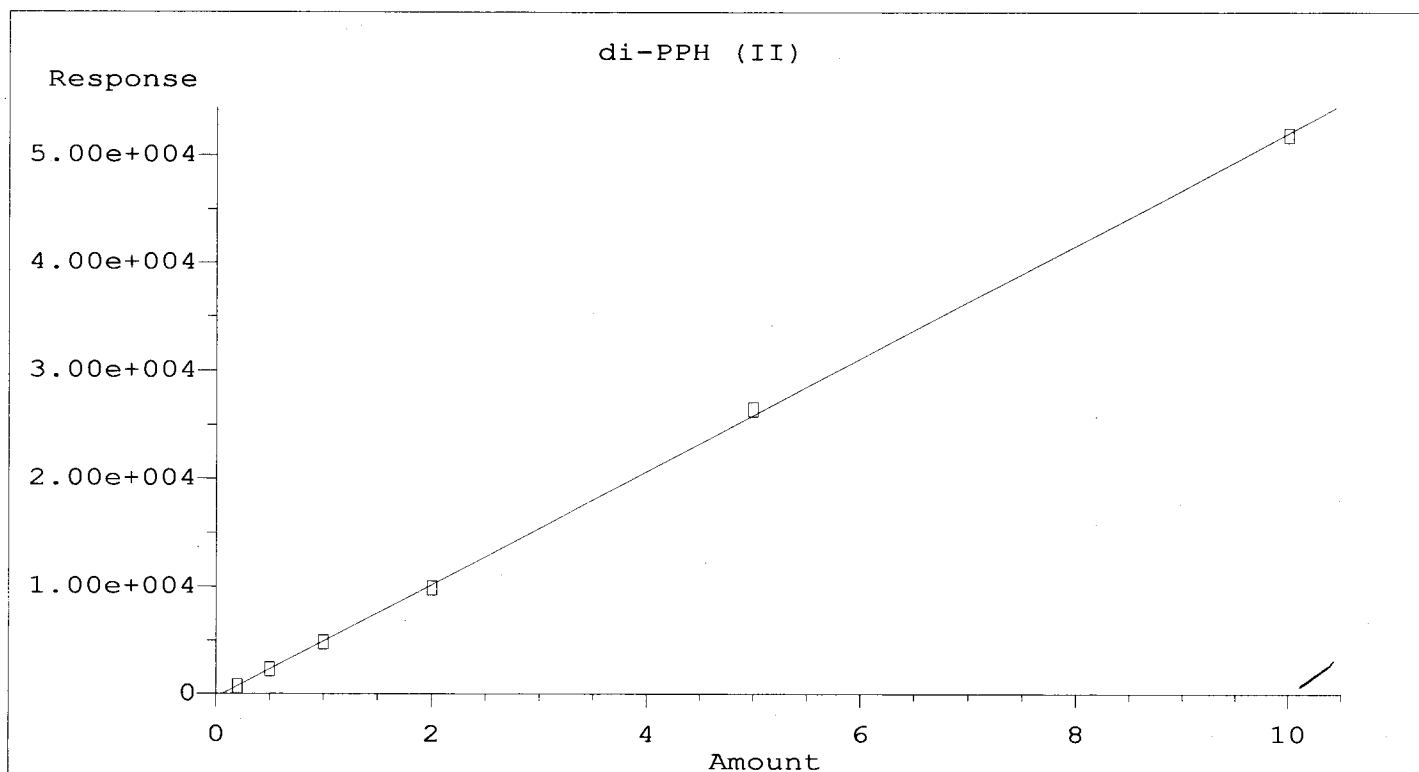


Response = $2.05e+004 * \text{Amt} + 7.64e+002$
 Coef of Det (r^2) = 0.999 Curve Fit: Linear

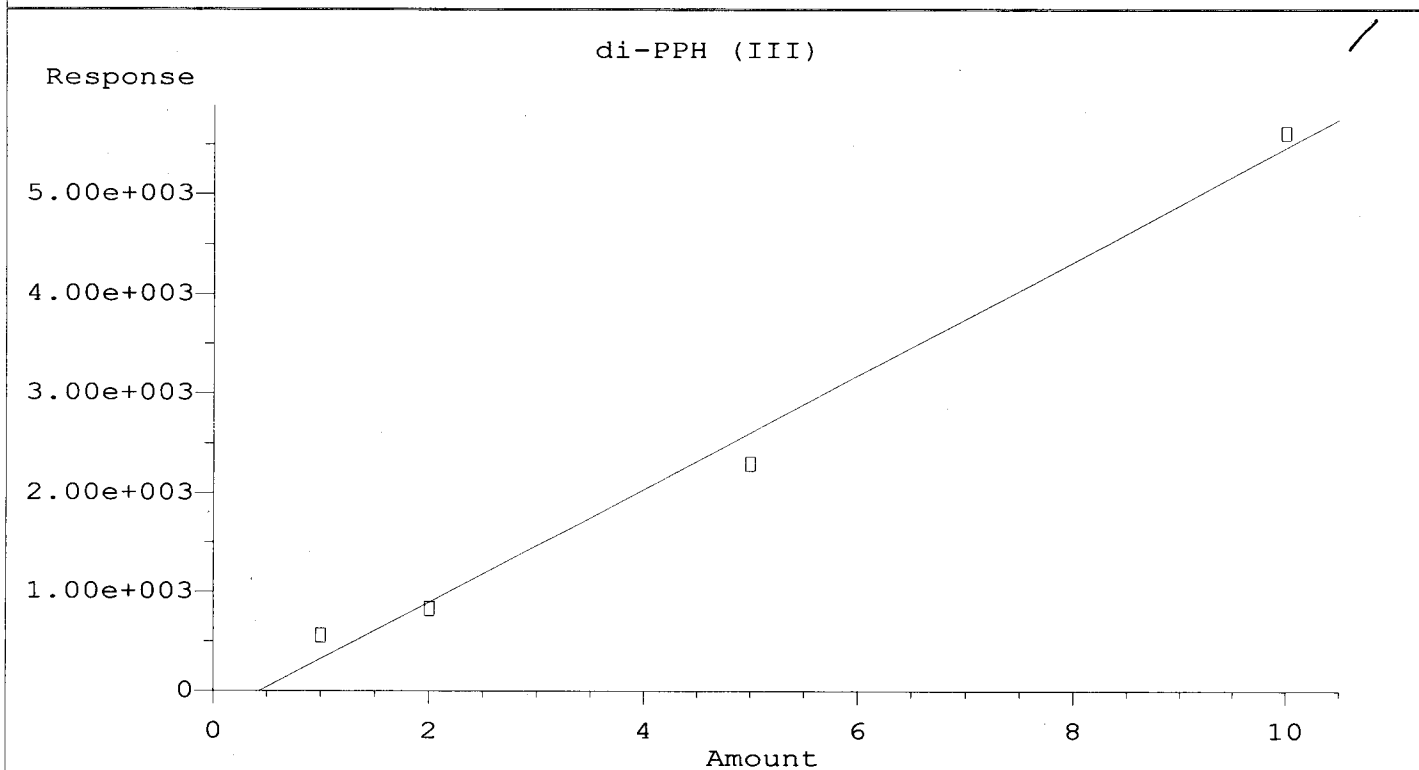


Response = $7.99e+003 * \text{Amt} - 2.84e+003$
 Coef of Det (r^2) = 0.998 Curve Fit: Linear

Calibration Plot Report

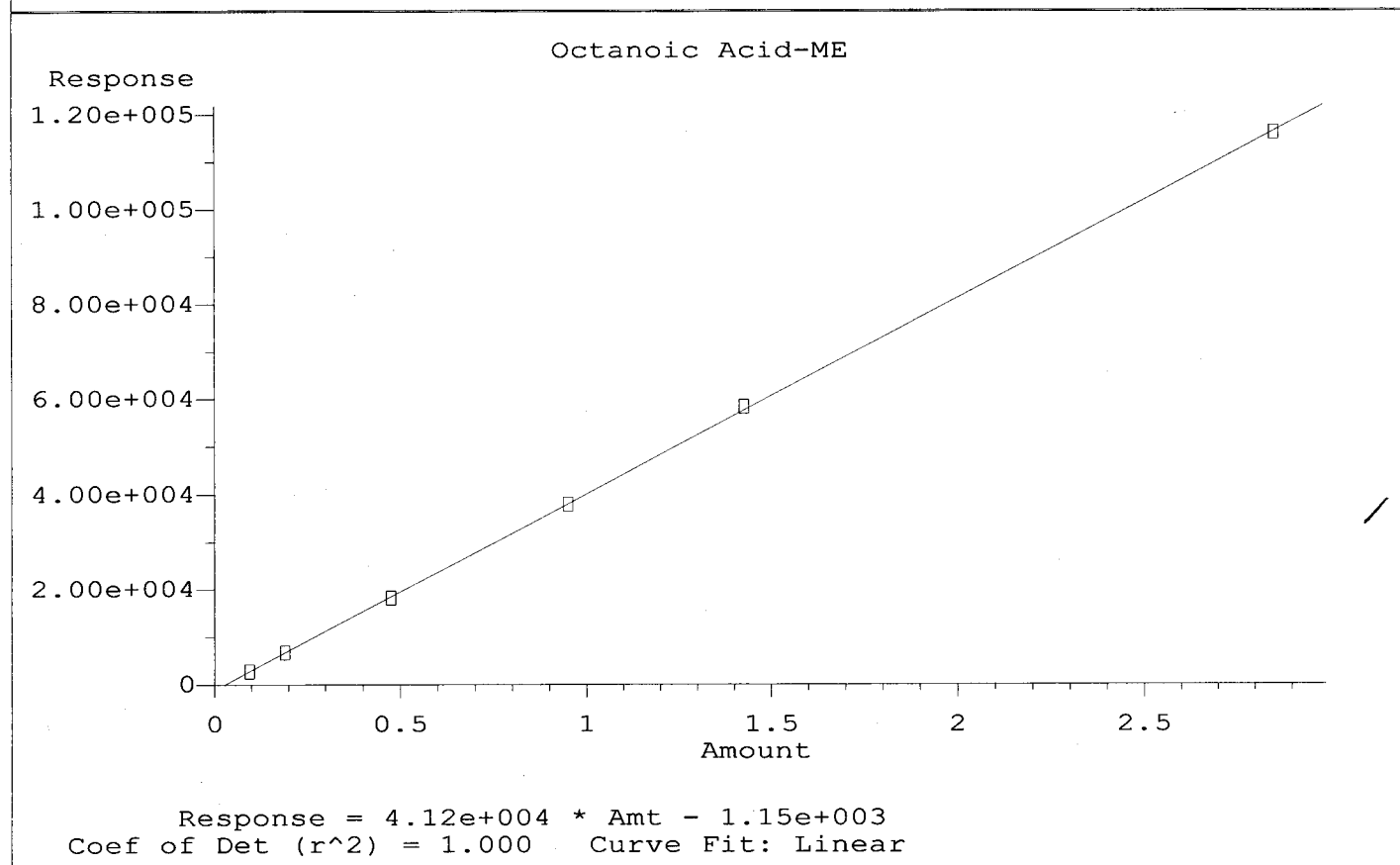
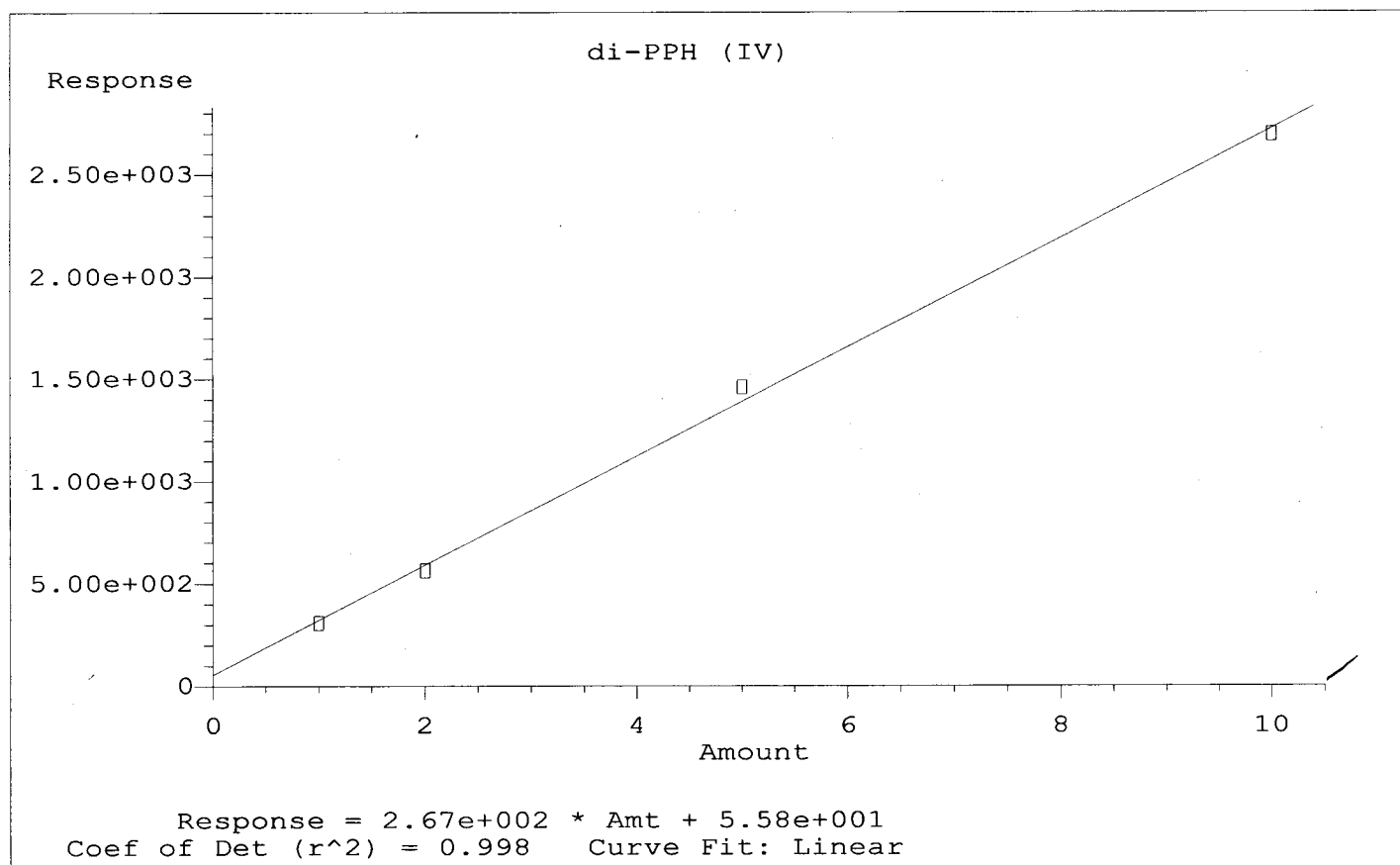


Response = $5.24e+003 * \text{Amt} - 3.35e+002$
 Coef of Det (r^2) = 1.000 Curve Fit: Linear

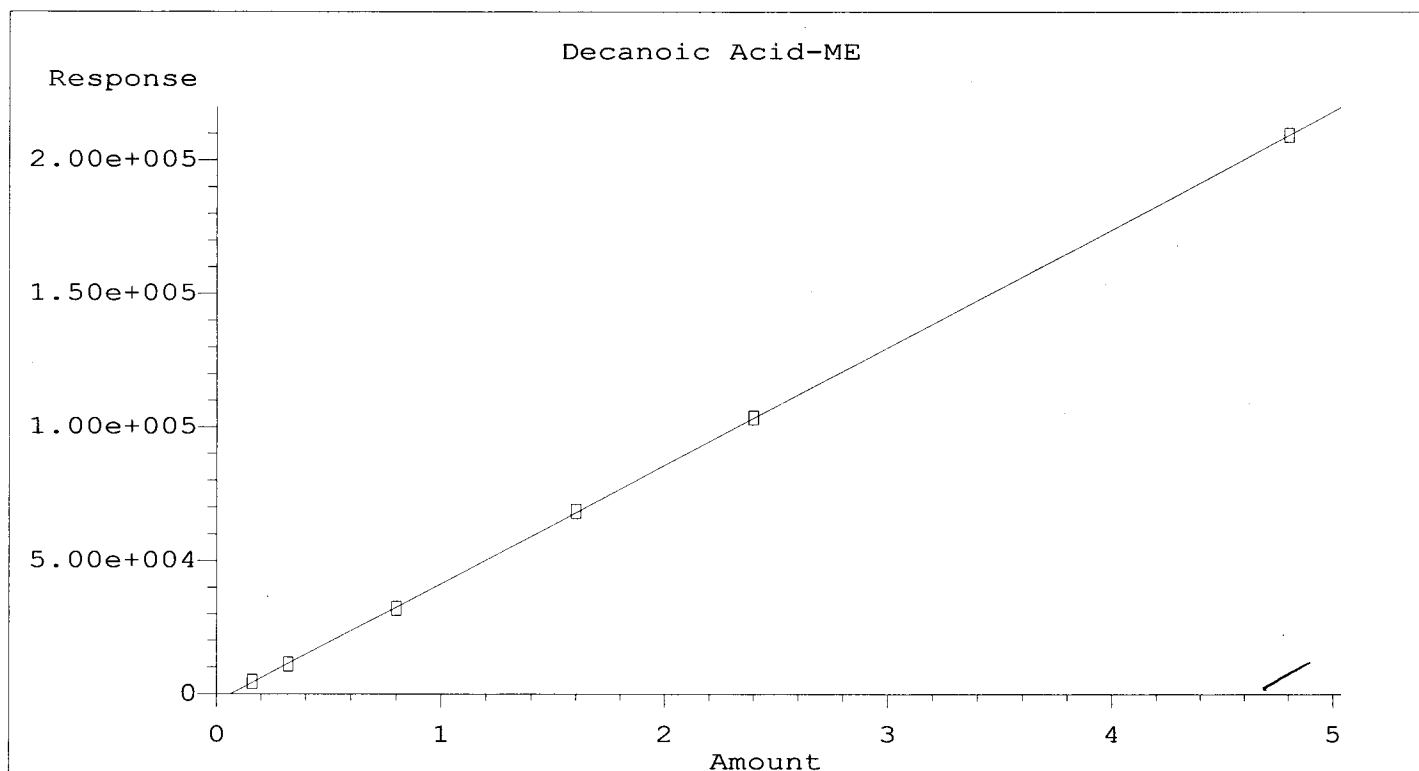


Response = $5.71e+002 * \text{Amt} - 2.44e+002$
 Coef of Det (r^2) = 0.989 Curve Fit: Linear

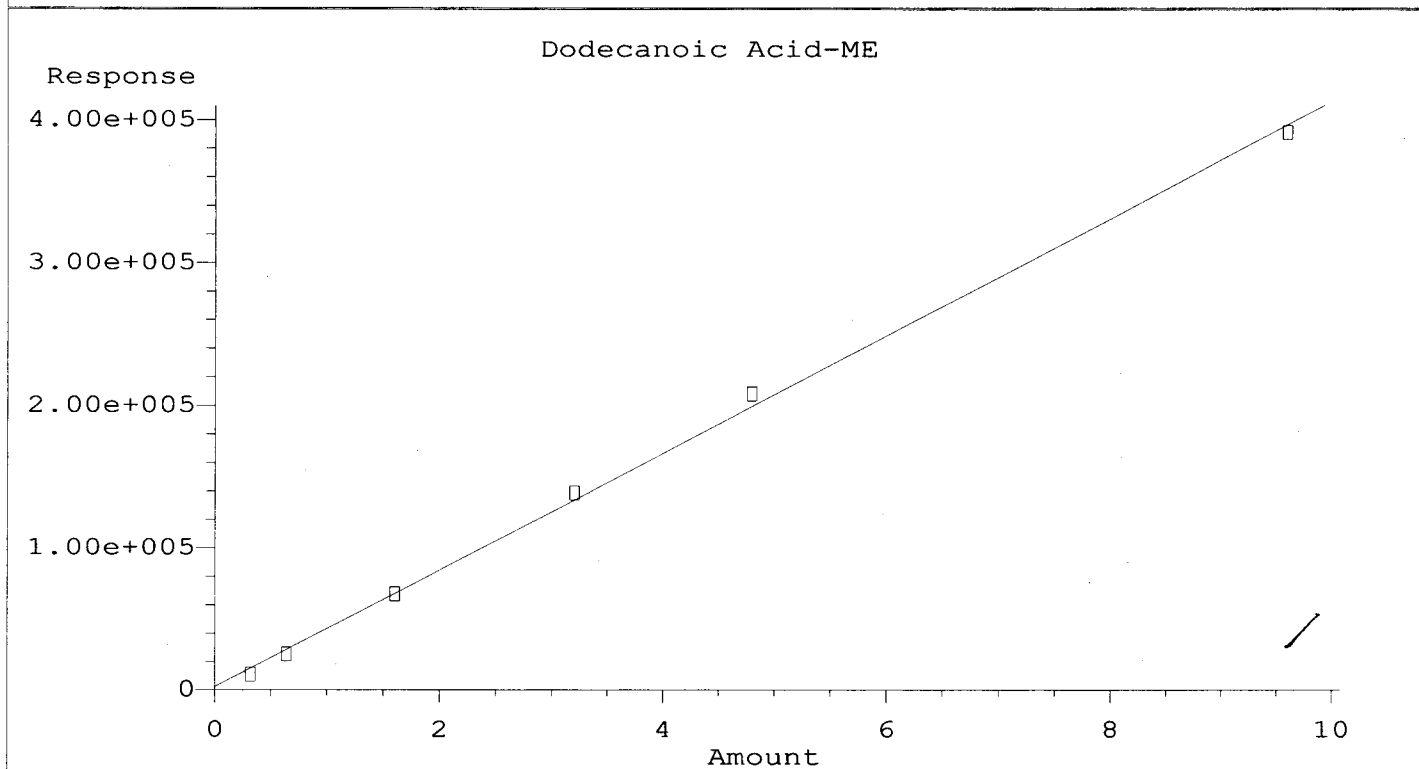
Calibration Plot Report



Calibration Plot Report

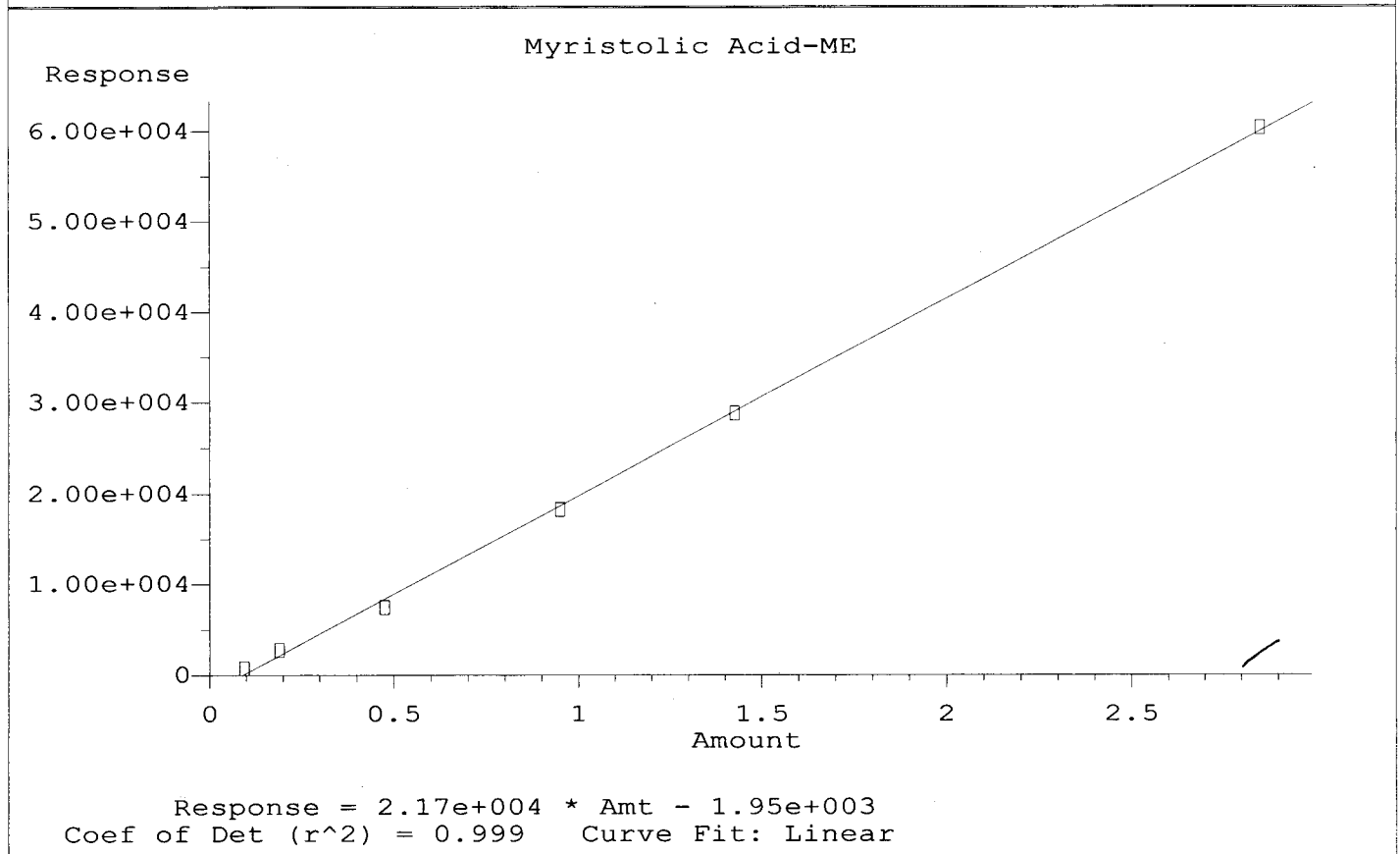
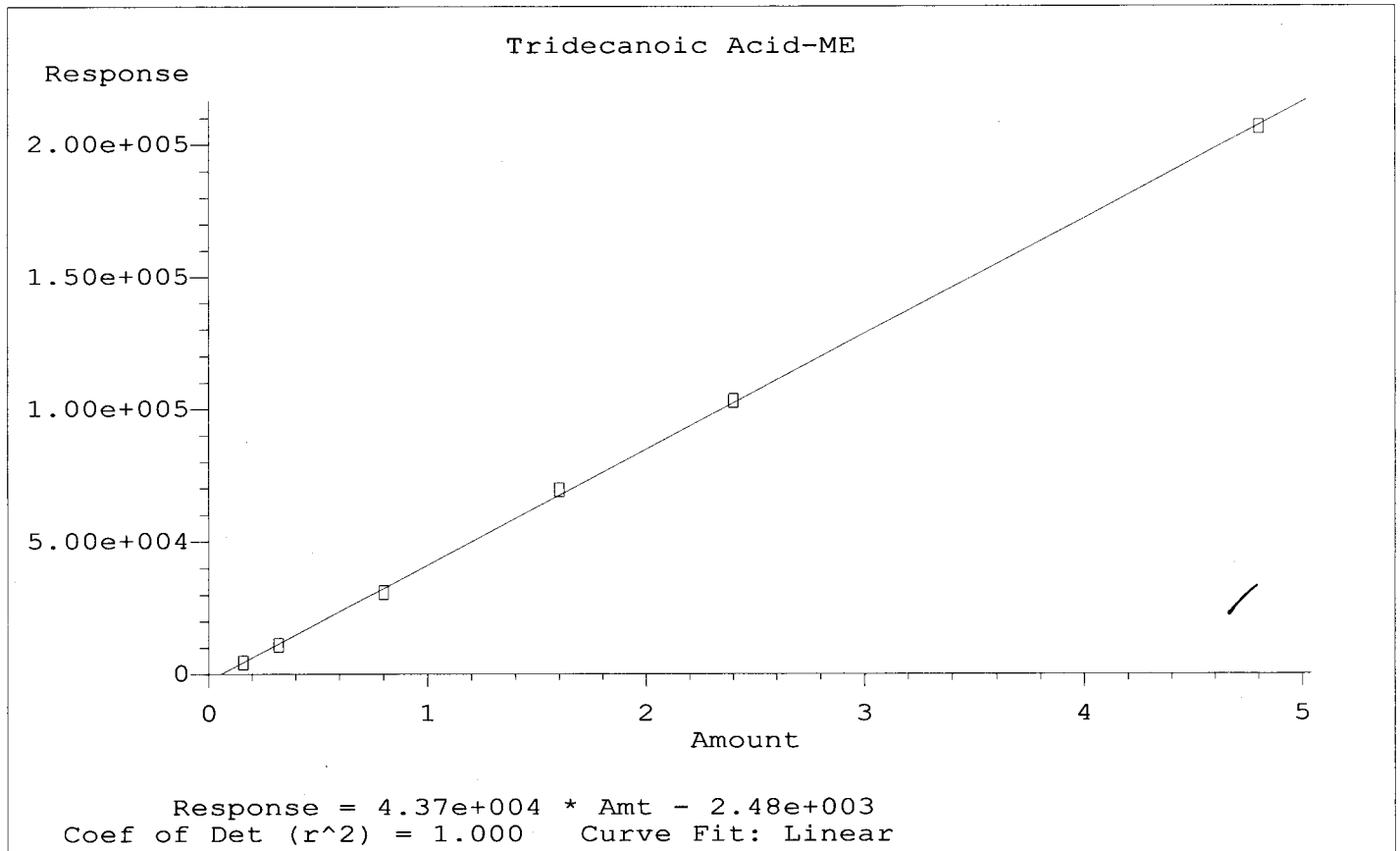


Response = $4.42 \times 10^4 \times \text{Amt} - 2.77 \times 10^3$
 Coef of Det (r^2) = 1.000 Curve Fit: Linear

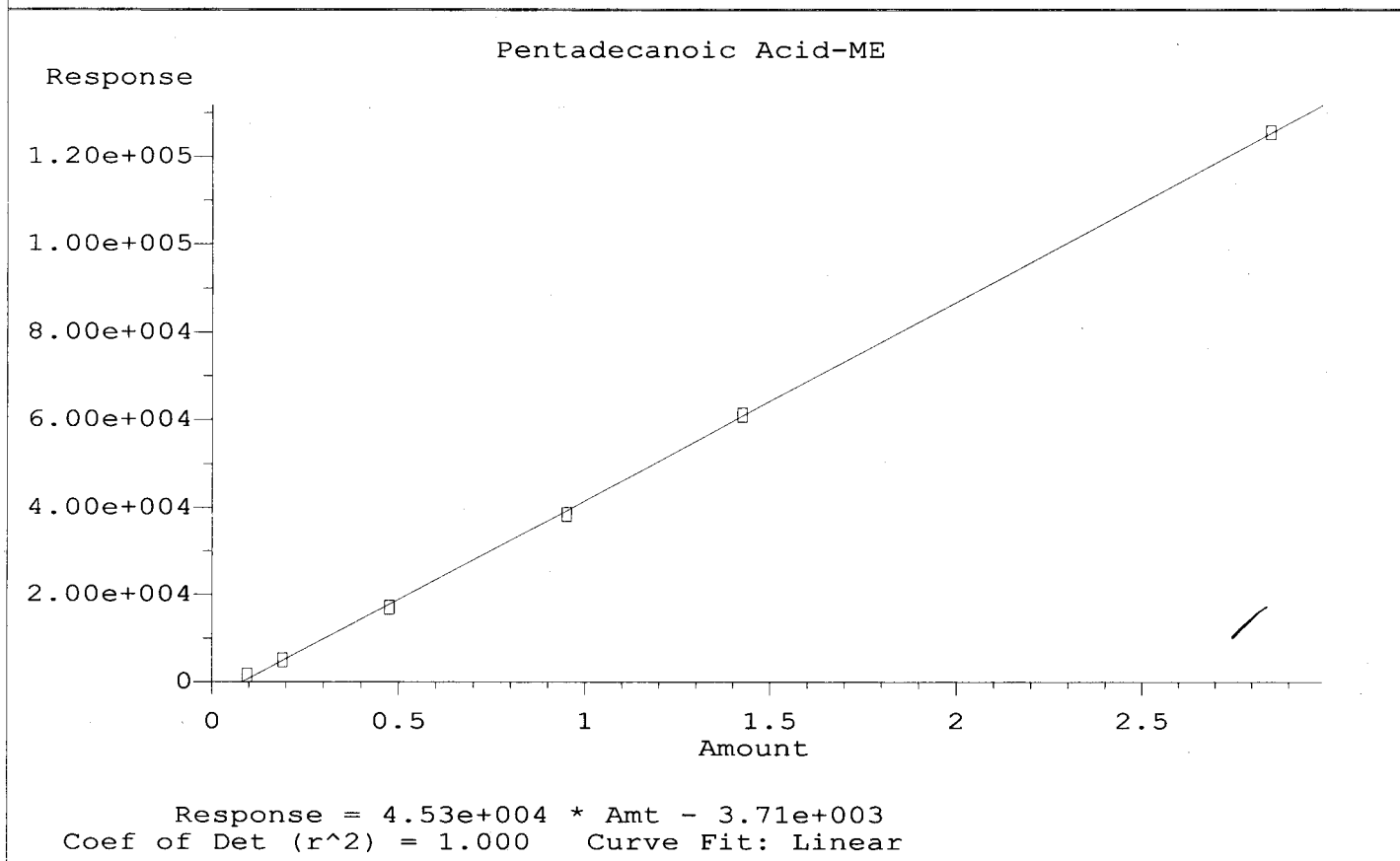
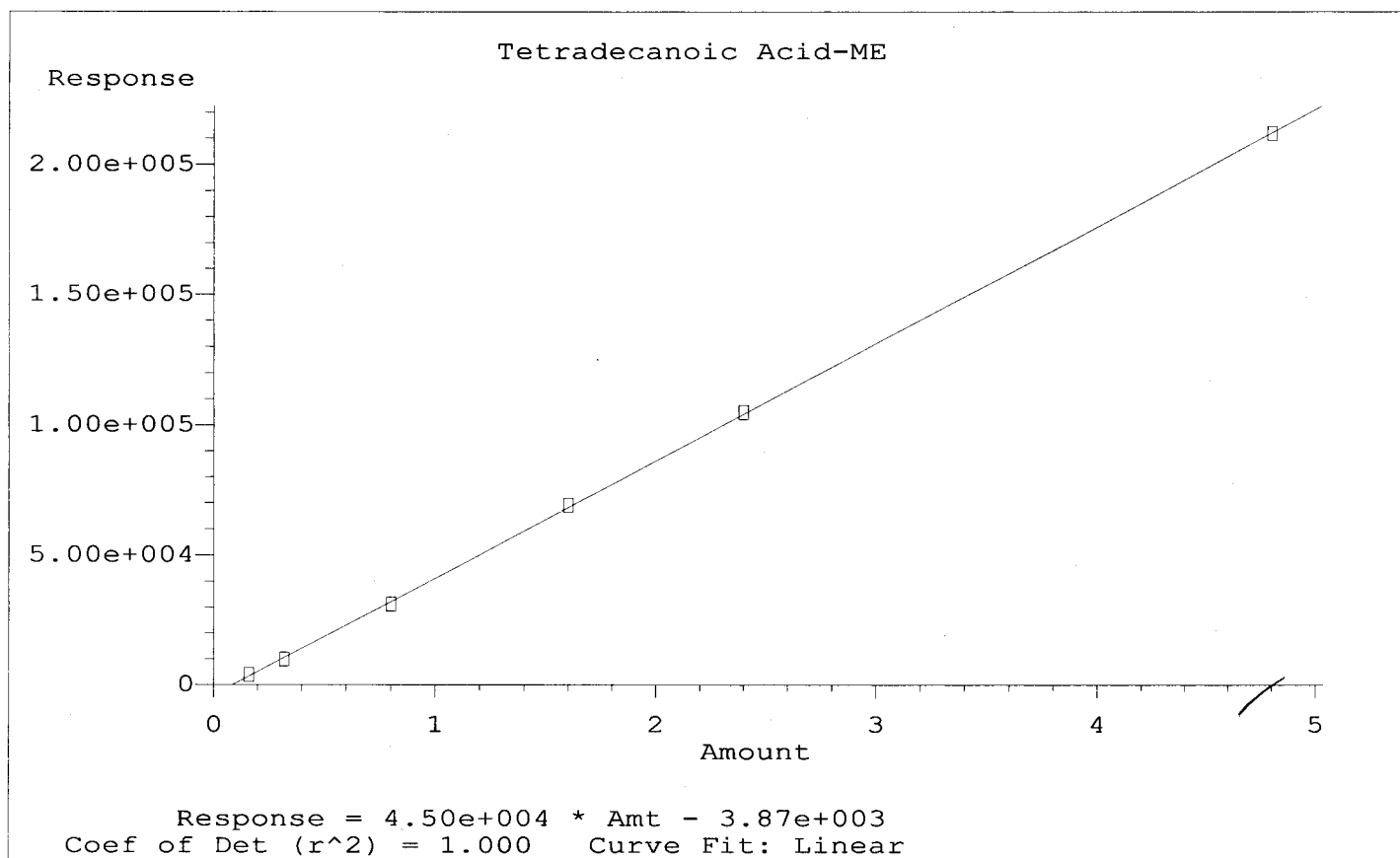


Response = $4.11 \times 10^4 \times \text{Amt} + 2.13 \times 10^3$
 Coef of Det (r^2) = 0.998 Curve Fit: Linear

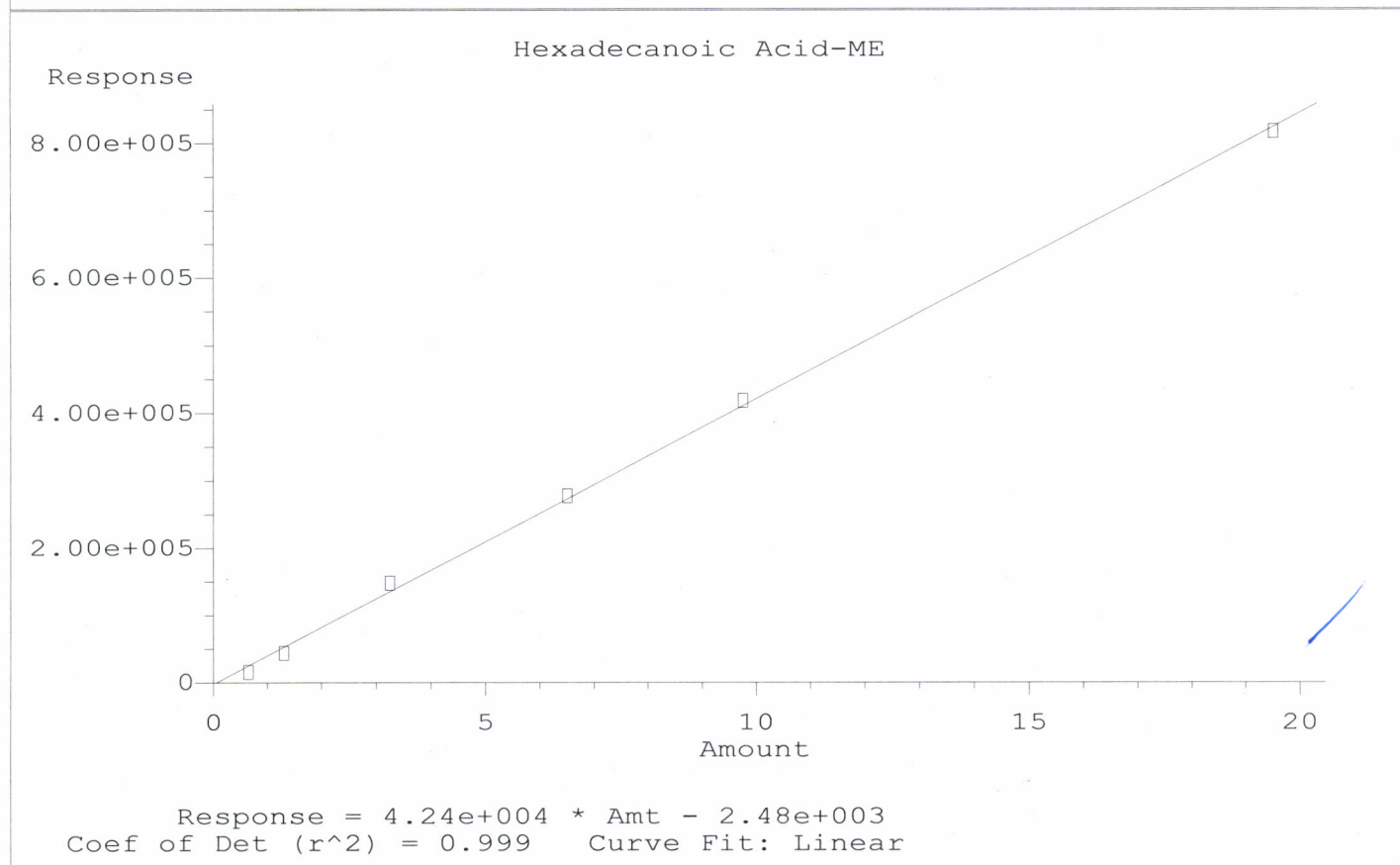
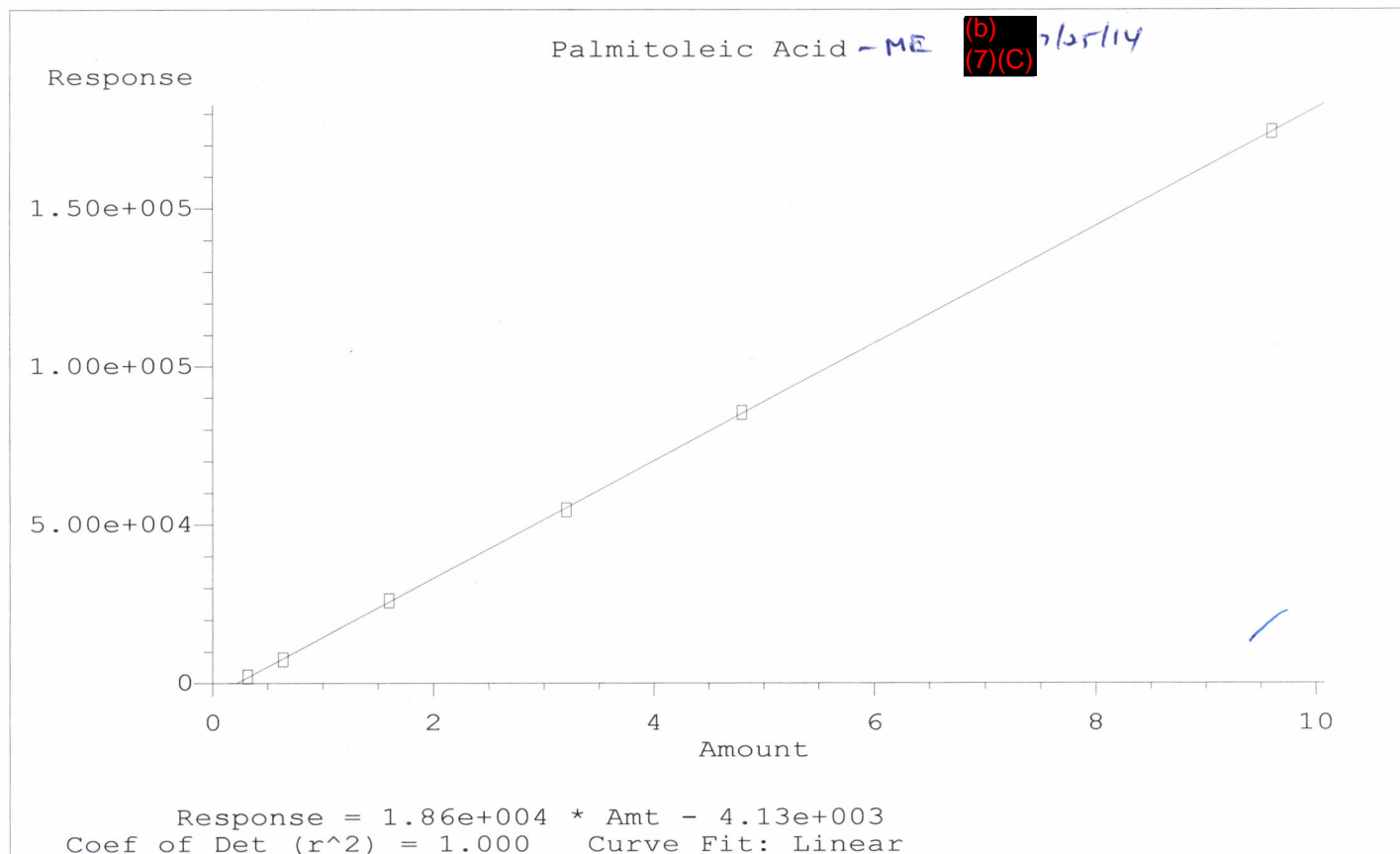
Calibration Plot Report



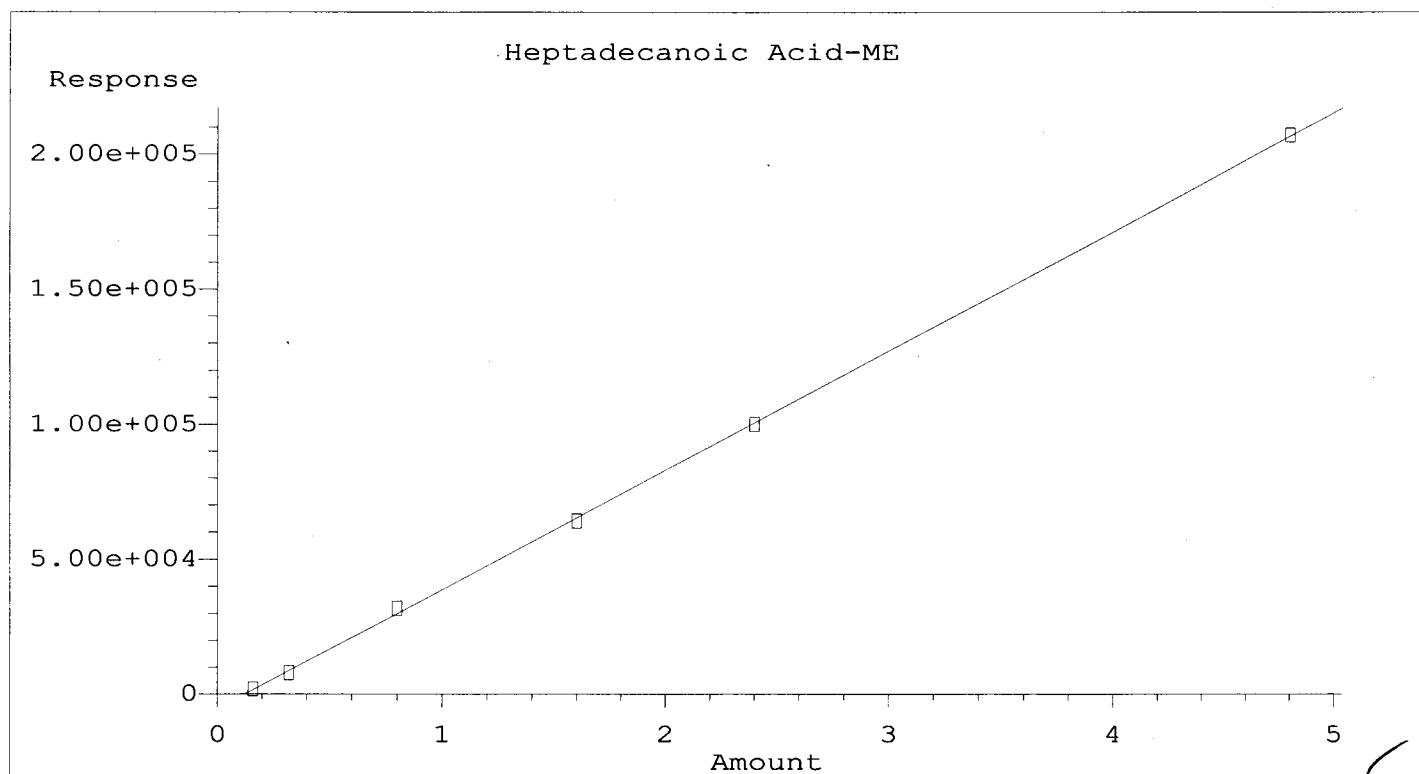
Calibration Plot Report



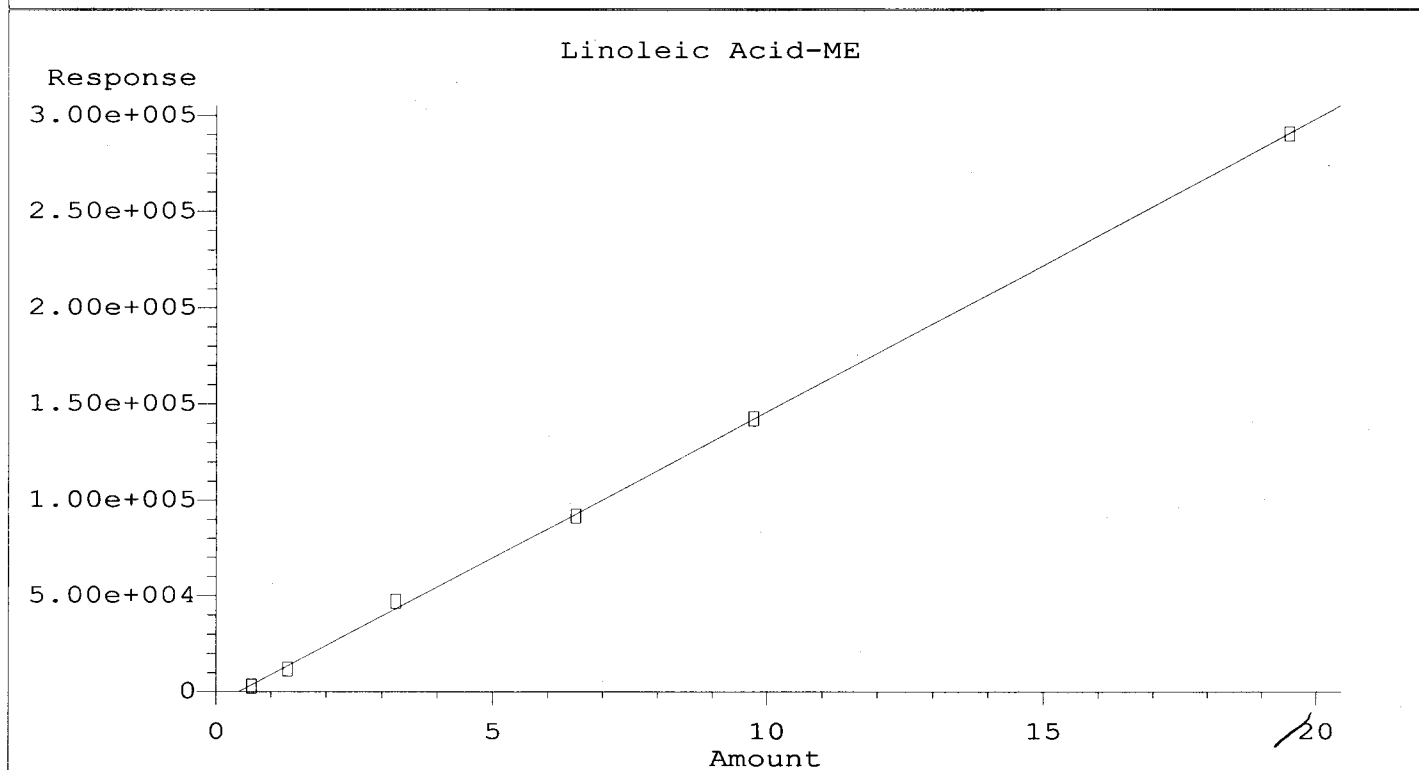
Calibration Plot Report



Calibration Plot Report

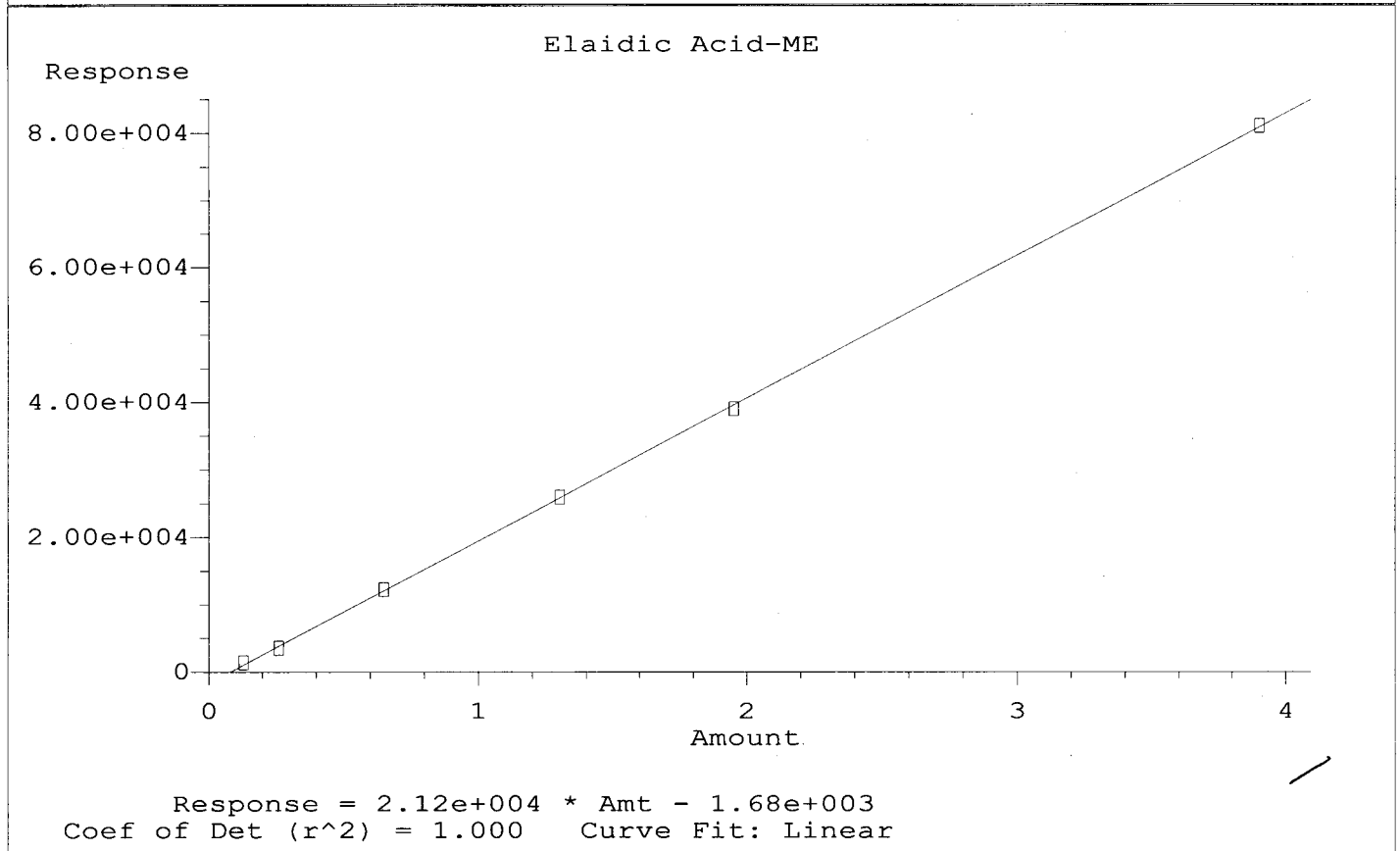
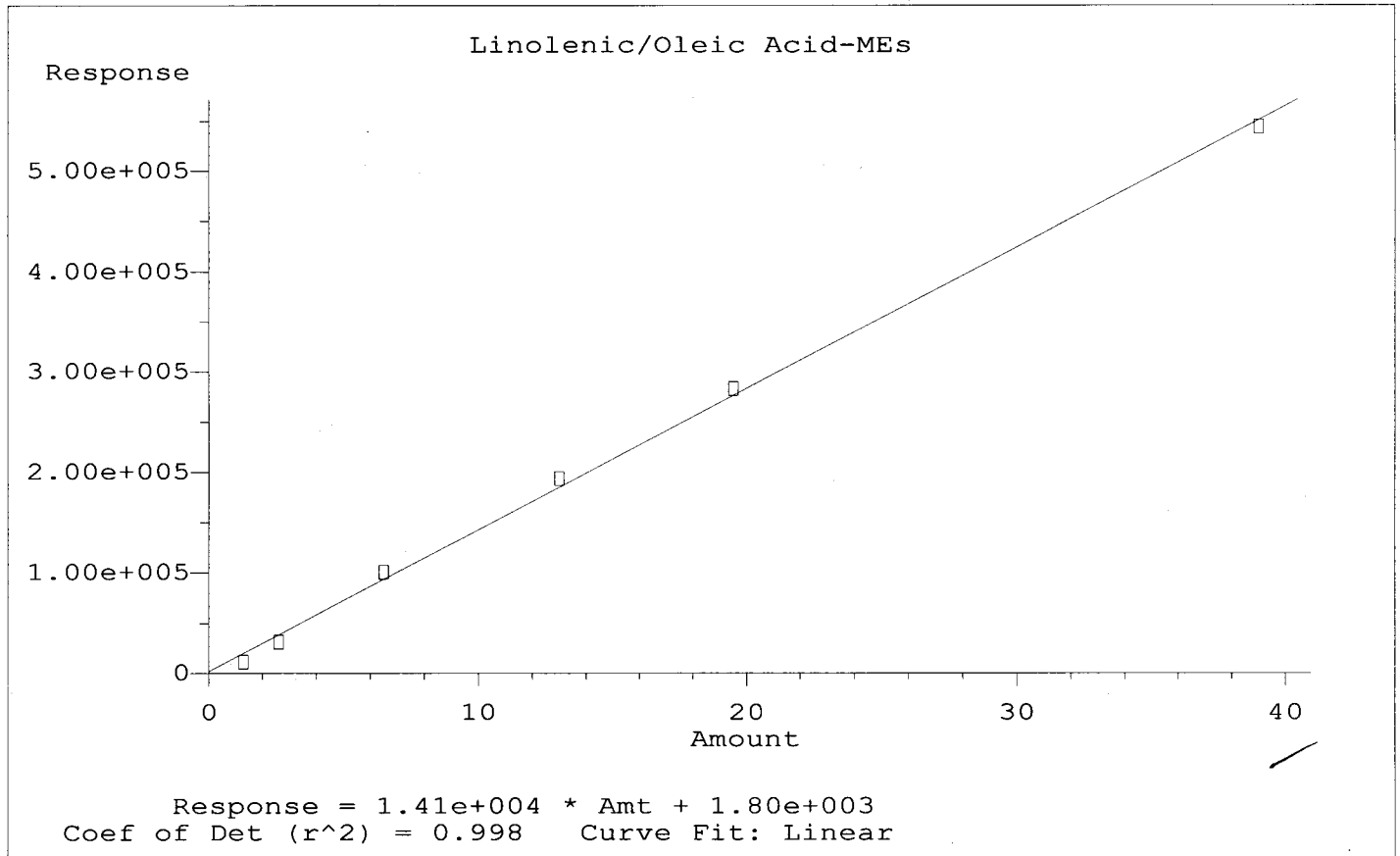


Response = 4.42×10^4 * Amt - 5.38×10^3
Coef of Det (r^2) = 1.000 Curve Fit: Linear

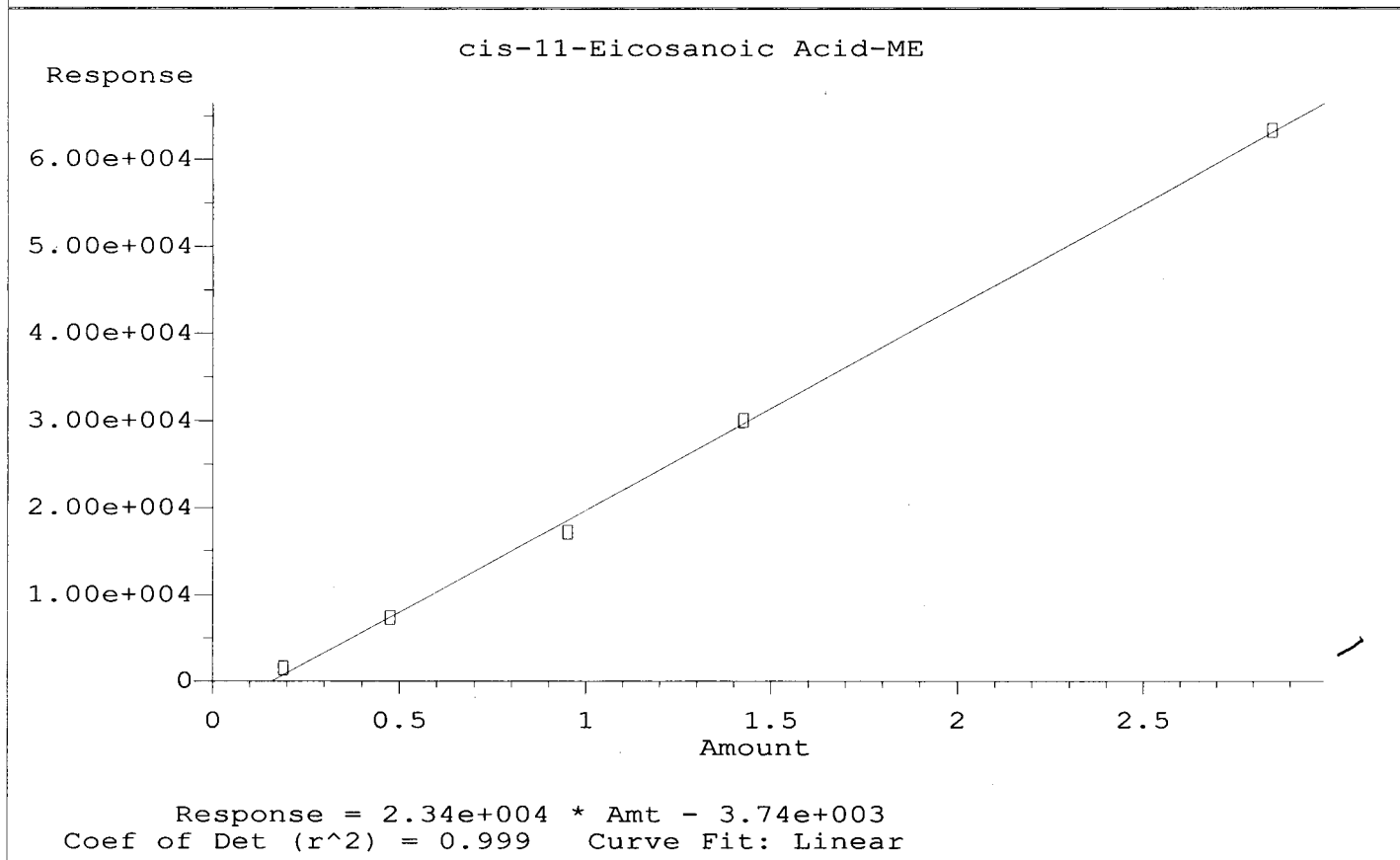
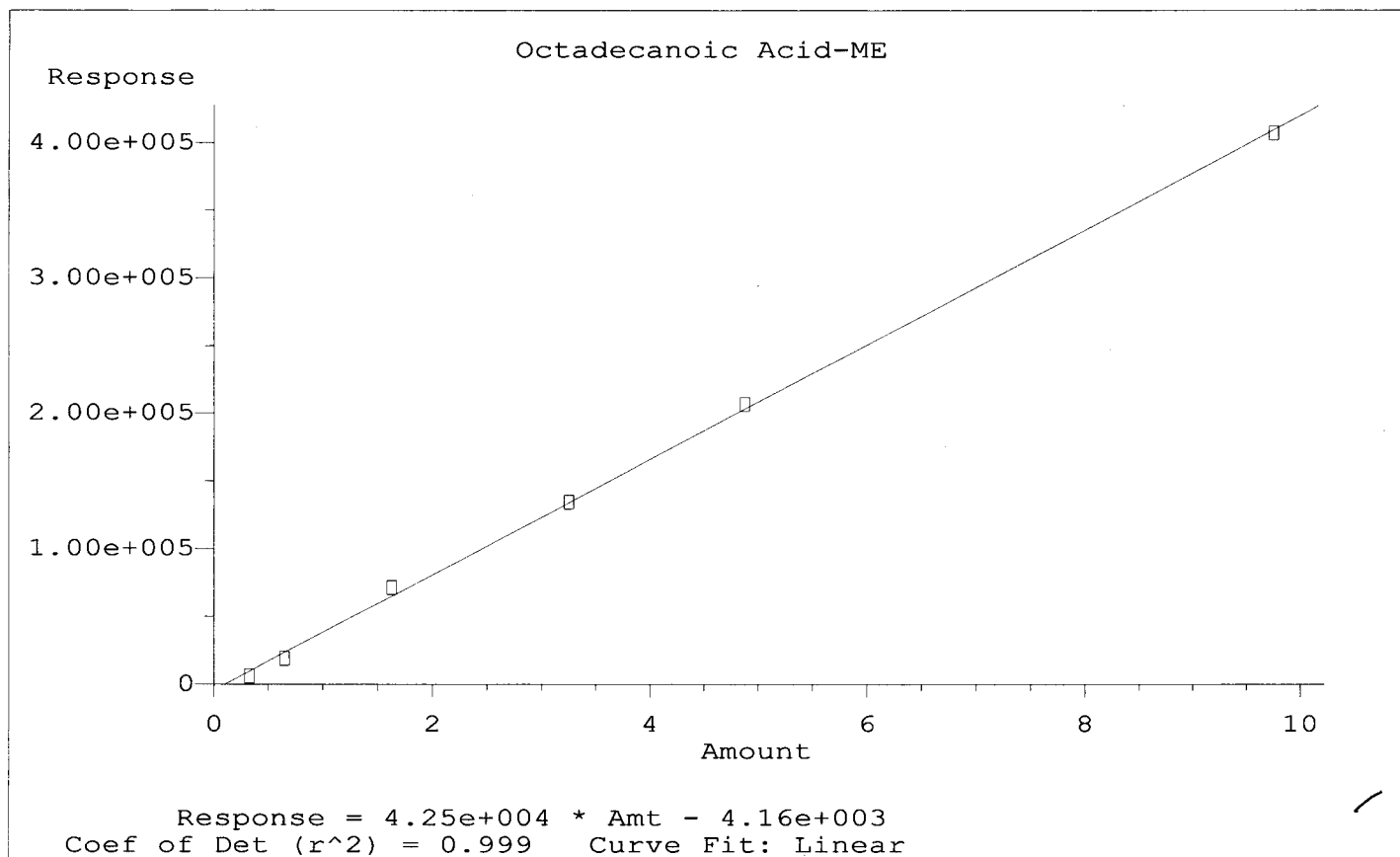


Response = 1.52×10^4 * Amt - 6.18×10^3
Coef of Det (r^2) = 1.000 Curve Fit: Linear

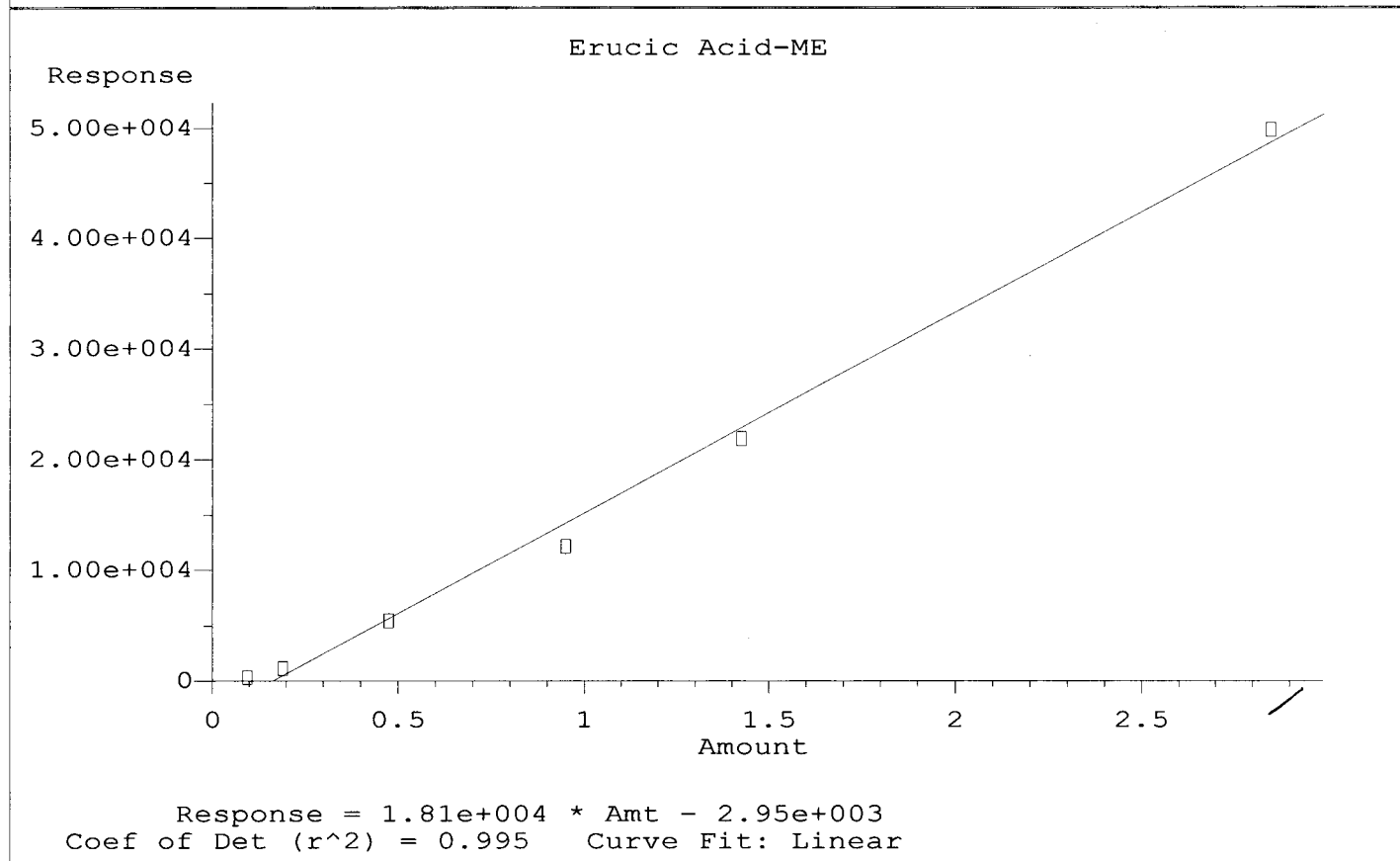
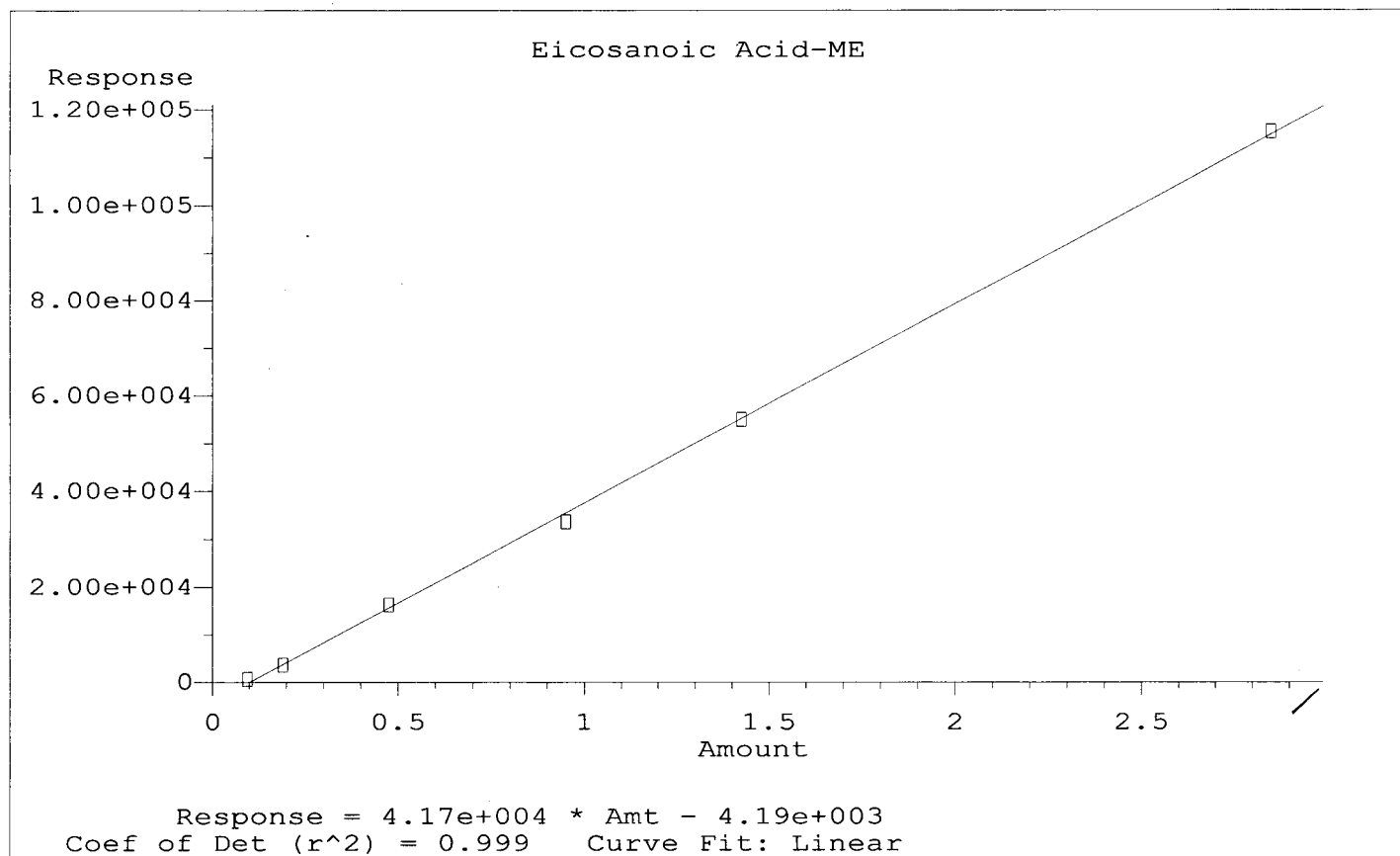
Calibration Plot Report



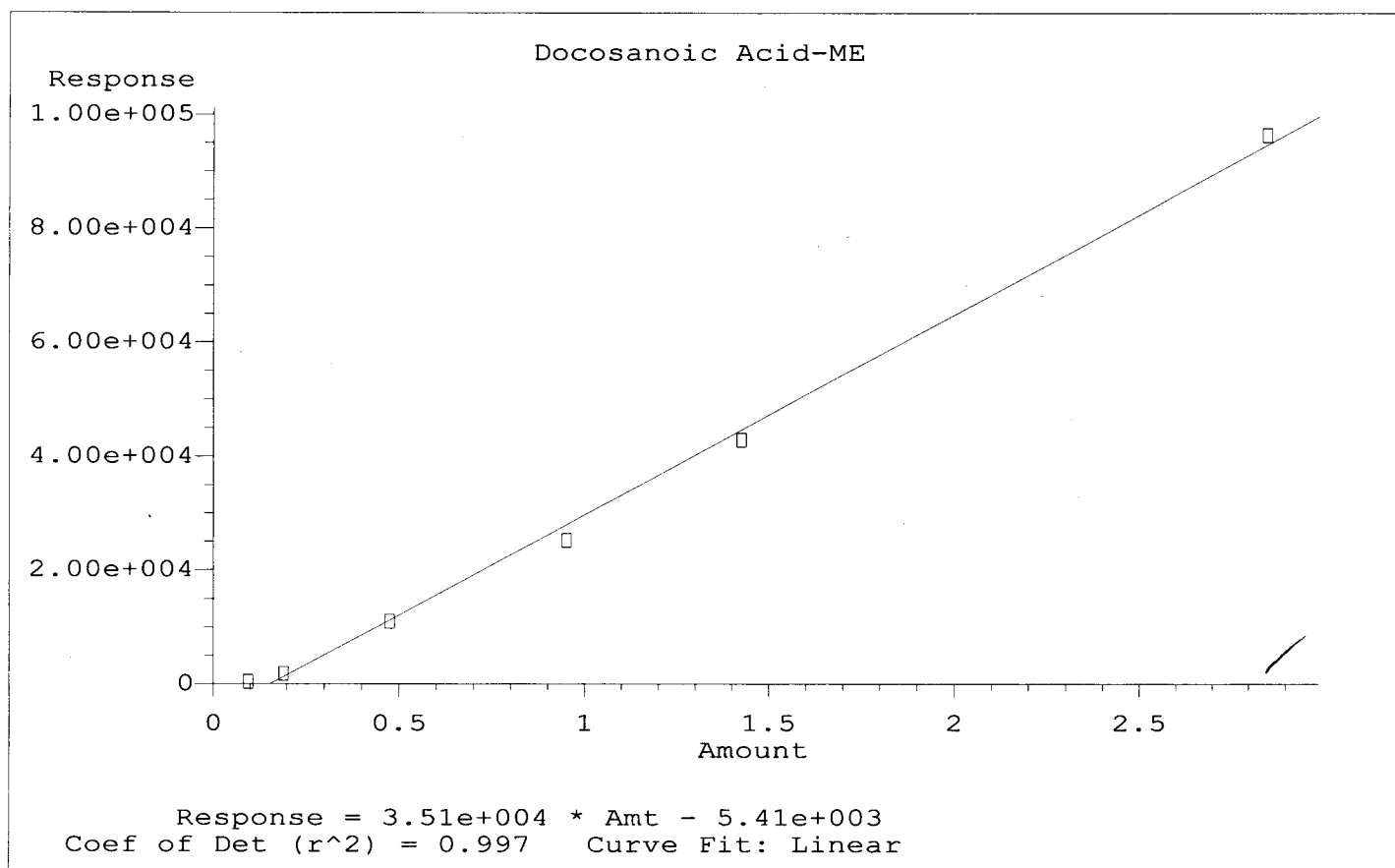
Calibration Plot Report



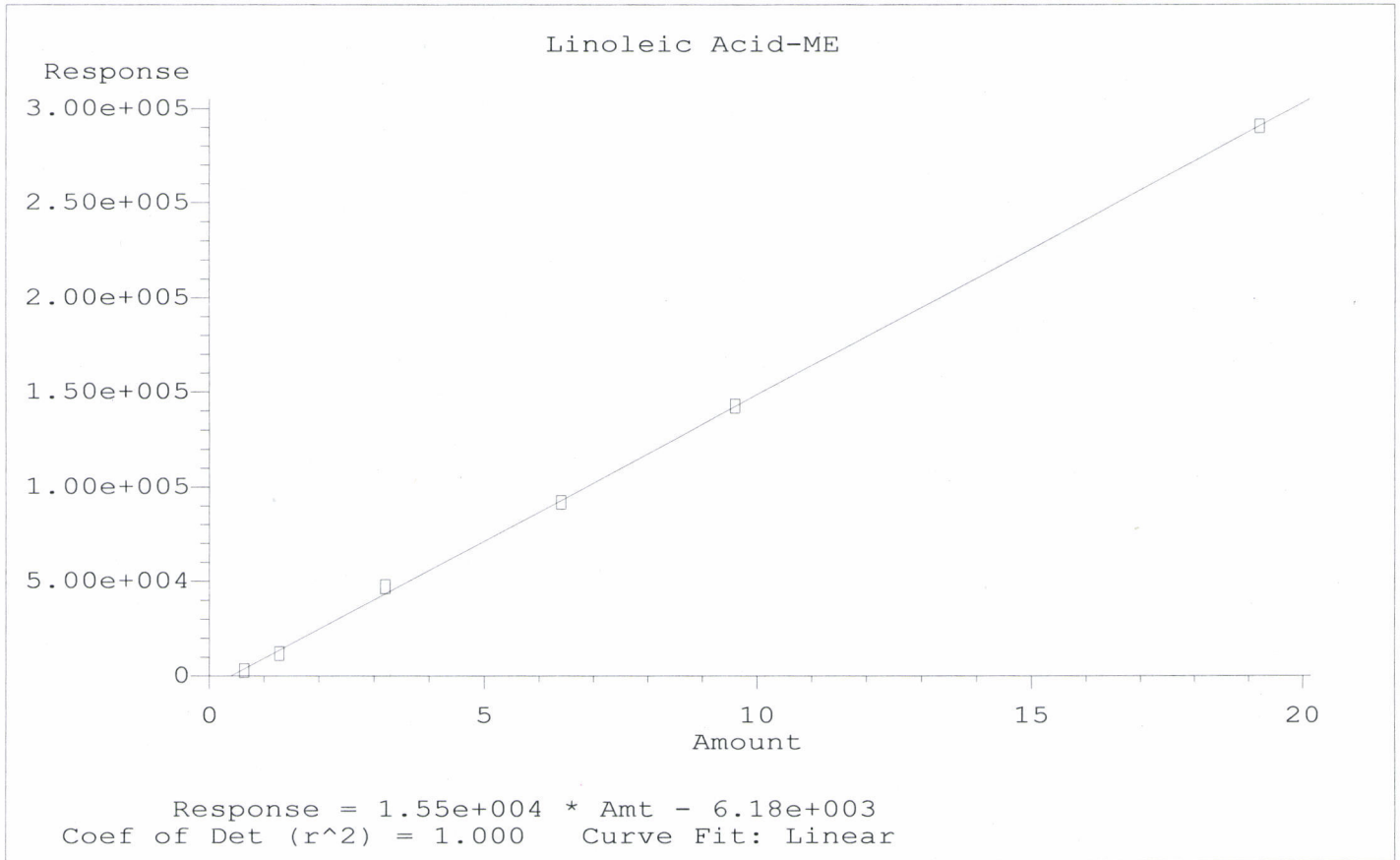
Calibration Plot Report



Calibration Plot Report



Calibration Plot Report



| <u>Lv</u> | <u>ID</u> | <u>[] $\frac{\mu g}{ml}$ *</u> | <u>Response</u> |
|-----------|-----------|--|-----------------|
| 1 | | 0.640 | 2760 |
| 2 | | 1.28 | 11912 |
| 3 | | 3.20 | 47002 |
| 4 | | 6.40 | 91893 |
| 5 | | 9.60 | 142337 |
| 6 | | 19.2 | 290518 |

Area Response for Linoleic acid-ME
 N405006-03 A = 269600

[Linoleic acid-ME]_{obs}

$$= \frac{269600 + 6180}{15500}$$

$$= 17.79 \frac{\mu g}{ml}$$

* [] values are based on
 a 12.8% weight % value.